Static Fission-Barrier Calculations of a Two-Parameter Liquid Drop*

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Calculations based on a two-parameter description of a uniformly charged liquid drop are reported. Results include fission-barrier energy and other saddle-point properties. The electrostatic energy of the drop was computed by a novel and highly accurate method. The saddle-point properties and corresponding drop shapes are compared with calculations that use nine parameters. Agreement is best for fissionability parameters greater than 0.70, suggesting that these calculations may provide a few-parameter basis for dynamical calculations of adequate precision at the larger fissionability parameters.

INTRODUCTION

SINCE the appearance in 1956 of Swiatecki's first paper of the series[1–5] entitled "The Deformation Energy of a Charged Drop," there has been an awakened interest in the theory of the liquid-drop model of nuclear fission. These papers provide the most complete description available to date of the static aspects of liquid-drop fission, including shapes described by as many as 18 parameters. More recently, similar results have been obtained by other authors[6–8] who solved an integro-differential equation to obtain the saddle-point shapes.

This paper describes static calculations of fission-barrier shapes and energies by means of a two-parameter family of algebraic expressions for the surface. Such calculations have two goals: (a) to synthesize as far as possible and simplify the results of Cohen and Swiatecki[5] in a few-parameter description, and (b) to provide the basis (in few parameters) for full dynamical calculations of the fission process. Kelson[9] and Nix[10] adopted similar programs based, however, on somewhat different families of shapes.

COULOMB AND SURFACE-ENERGY CALCULATIONS

We consider the family of surfaces described in cylindrical coordinates by

$$\rho^2 = aZ^4 + bZ^2 + c, \tag{1}$$

which form was suggested by the saddle-point shapes obtained in Ref. 5. The requirement of constant volume is utilized to eliminate the constant c, so that Eq. (1) describes a two-parameter family of possible shapes at the fission barrier.

The cylindrical coordinate system chosen for representing the drop permits a particularly simple expression for the Coulomb energy, which is quite suitable for modern digital computers. The Coulomb energy E_C of the volume of revolution is expressed as a double integration over the interaction energy of infinitely many disks, into which the volume may be decomposed.

Gray[11] obtained a general Bessel function expression for the electrostatic potential at a point due to a thin disk of uniform charge density σ. Integrating his expression appropriately over a similar coaxial disk yields the Coulomb interaction energy of the pair:

$$E_{C \text{ disks}} = 2\pi^2\sigma^2 dZ_A dZ_B$$

$$\times \int_0^\infty e^{-\lambda|Z_A - Z_B|} J_1(\lambda\rho_A) J_1(\lambda\rho_B)\frac{d\lambda}{\lambda^2}. \tag{2}$$

This expression was integrated with respect to Z_A and Z_B over the full range of Z to give the total Coulomb energy of the drop. The resulting Bessel function integral was converted to an integral of trigonometric functions by use of Watson's identity.[12] Expressed relative to the Coulomb energy of a sphere $E_C{}^0$, the actual integral evaluated is

$$B_C = \frac{E_C}{E_C{}^0} = 120 Z_0{}^5 \int_0^1 \rho_1{}^2 dz \int_0^1 z\rho_2{}^2 dy \int_0^1 \frac{\sin^2\pi w\, dw}{z(1-y) + [z^2(1-y)^2 + \rho_1{}^2 + \rho_2{}^2 - 2\rho_1\rho_2\cos\pi w]^{1/2}}, \tag{3}$$

[1] W. J. Swiatecki, Phys. Rev. 101, 651 (1956).
[2] W. J. Swiatecki, Phys. Rev. 104, 993 (1956).
[3] W. J. Swiatecki, *Proceedings of the Second United Nations International Conference on the Peaceful Uses of Atomic Energy, Geneva, 1958* (United Nations, Geneva, 1958), Vol. 15, p. 248.
[4] S. Cohen and W. J. Swiatecki, Ann. Phys. 19, 67 (1962).
[5] S. Cohen and W. J. Swiatecki, Ann. Phys. 22, 406 (1963).
[6] V. M. Strutinskiĭ, Zh. Eksperim. i Teor. Fiz. 42, 1571 (1962) [English transl.: Soviet Phys.—JETP 15, 1091 (1962)].
[7] V. M. Strutinskiĭ, N. Ya. Lyashchenko, and N. A. Popov, Zh. Eksperim. i Teor. Fiz. 43, 584 (1962) [English transl.: Soviet Phys.—JETP 16, 418 (1963).
[8] V. M. Strutinskiĭ, *Results of Calculations Based on the Liquid Drop Model of Nuclear Fission* (Order of Lenin, Institute of Atomic Energy, Moscow, 1963).
[9] I. Kelson, Phys. Rev. 136, B1677 (1964).
[10] J. R. Nix, Lawrence Radiation Laboratory Report No. UCRL-11338, 1964 (unpublished).
[11] A. Gray, Phil. Mag. 38, 201 (1919).
[12] G. N. Watson, *A Treatise on the Theory of Bessel Functions,* (University Press, Cambridge, England, 1944), p. 389, 13.22(1).

TABLE I. Calculated values of relative Coulomb and surface energies of a sphere and two spheroids, with comparable figures for other investigators.

Machine or author	Gauss order or number of grid points	Sphere	Spheroid $\dfrac{\text{Major axis}}{\text{Minor axis}} = \dfrac{1}{0.7}$	Spheroid $\dfrac{\text{Major axis}}{\text{Minor axis}} = \dfrac{1}{0.5}$
		Relative Coulomb energy B_C		
STRETCH	Exact[a]	1.000 000 000	0.988 678 870	0.957 975 925
STRETCH	16	0.999 999 707	0.988 678 577	0.957 975 557
STRETCH	96	0.999 999 998	0.998 678 869	0.957 975 925
Cohen and Swiatecki[b]	41	0.999 998 2	0.988 676 6	...
Cohen and Swiatecki[b]	61	0.999 999 3	0.988 678 4	...
Cohen and Swiatecki[b]	81	...	0.988 678 6	...
Beringer[c]	40	0.999 828	...	0.957 662
		Relative surface energy B_S		
STRETCH	Exact[a]	1.000 000 000	1.021 383 583	1.076 728 262
STRETCH	16	1.000 000 000	1.021 383 583	1.076 728 262
STRETCH	96	1.000 000 000	1.021 383 583	1.076 728 262

[a] "Exact" means that the closed algebraic expressions for the energies were evaluated, while the numbers designate numerical integrations.
[b] Reference 5.
[c] Reference 14.

where

$$\rho_1{}^2 = 4aZ_0{}^2z^4 - 8aZ_0{}^2z^3 + (6aZ_0{}^2+b)z^2 - (2aZ_0{}^2+b)z,$$

$$\rho_2{}^2 = 4aZ_0{}^2z^4y^4 - 8aZ_0{}^2z^3y^3 + (6aZ_0{}^2+b)z^2y^2 - (2aZ_0{}^2+b)zy,$$

and $2Z_0$ is the length of the drop at $\rho=0$.

The integral representation of the surface energy relative to that of a sphere $E_S{}^0$ is

$$B_S = \frac{E_S}{E_S{}^0} = Z_0 \int_0^1 [4a^2Z_0{}^6u^6 + (4ab+a)Z_0{}^4u^4 + (b^2+b)Z_0{}^2u^2+c]^{1/2}du. \quad (4)$$

Equations (3) and (4) were evaluated on the IBM 7030 (STRETCH) computer by Legendre-Gauss quadrature.[13] This integration technique was chosen because it has a precision of order $2N-1$ when only N evaluation points are used. In common with all numerical integration schemes, more accurate results can be obtained by using a larger number of evaluation points (higher order quadrature) at the cost, of course, of more computational time.

The triple Coulomb integrals were evaluated for the sphere and two spheroids, using 16th- and 96th-order Legendre-Gauss quadrature. In Table I these results are compared to the exact energies for these shapes and with the results of Cohen and Swiatecki[5] and Beringer.[14] The 16th-order quadrature is seen to be accurate to four parts in 10^7, meeting or exceeding the accuracy of previous calculations. While the 96th-order Gauss quadrature was slightly more accurate, each triple integration required 6 min of computer time compared with 3 sec for the 16th-order quadrature.

Table I also includes the single Gauss quadrature

[13] F. B. Hildebrand, Introduction to Numerical Analysis (McGraw-Hill Book Company, Inc., New York, 1956), p. 312.
[14] R. Beringer, Phys. Rev. 131, 1402 (1963).

results for the relative surface energy B_S. Both the 16th- and the 96th-order quadrature are seen to be in precise agreement with the exact evaluations for the indicated number of significant digits. These calculations, therefore, establish the accuracy and desirability of the 16th-order Gauss quadrature, which was used to compute the final results.

SADDLE-POINT DETERMINATION

The classical fission threshold is represented by the saddle point of the relative deformation energy ξ:

$$\xi = B_S - 1 + 2x(B_C - 1), \quad (5)$$

where $x = E_C{}^0/2E_S{}^0$, and is the Bohr and Wheeler fissionability parameter.[15] For a function of two variables such as $\xi(a,b)$, a saddle point is mathematically defined to be a point (a_{SP}, b_{SP}) in the vicinity of which the first and second partial derivatives are continuous and at which (a) the two first partial derivatives are zero and (b) the second partial derivatives satisfy the relation[16]

$$\left(\frac{\partial^2\xi}{\partial a\partial b}\right)^2 - \frac{\partial^2\xi}{\partial a^2}\frac{\partial^2\xi}{\partial b^2} > 0. \quad (6)$$

In the neighborhood of the saddle point, the contour of the deformation-energy hypersurface is approximated by a quadratic expression in the parameters. The saddle point is then obtained by computing the deformation energy, Eq. (5), in a grid of points near the saddle, and

[15] N. Bohr and J. A. Wheeler, Phys. Rev. 56, 426 (1939).
[16] If condition (b) is not satisfied, the point located by condition (a) may be a maximum, minimum, or inflection point. Two nonsaddle cases arise in the present calculations: (1) When $x < 1.00$, the spherical configuration is a minimum of the deformation energy. (2) When $x = 1.00$, the saddle point and minimum coalesce, and the result is an inflection point.

mathematically fitting the "best" quadratic surface to these energies.

The quadratic approximation in the vicinity of the saddle point is

$$\xi(a,b) = C_1 + C_2 a + C_3 b + C_4 a^2 + C_5 ab + C_6 b^2. \quad (7)$$

When the coefficients satisfy Eq. (6) (i.e., $C_5^2 - 4C_4C_6 > 0$), the saddle point is

$$a_{SP} = (C_3 C_5 - 2C_2 C_6)/(4C_4 C_6 - C_5^2),$$
$$b_{SP} = (C_2 C_5 - 2C_3 C_4)/(4C_4 C_6 - C_5^2). \quad (8)$$

Six points in the parameter space are needed to determine the coefficients $(C_j, \; j = 1, 6)$ of Eq. (7). A pentagonal grid was chosen surrounding an initial estimate of the saddle point (a_i, b_i). The deformation energy ξ was calculated for each of these six point sets. A matrix
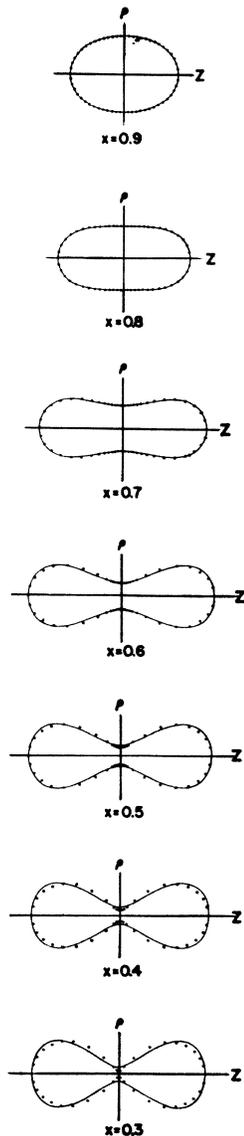
FIG. 1. Comparison of saddle-point shapes as calculated in a two-parameter space (continuous line) with those of Ref. 5 (designated by ●).
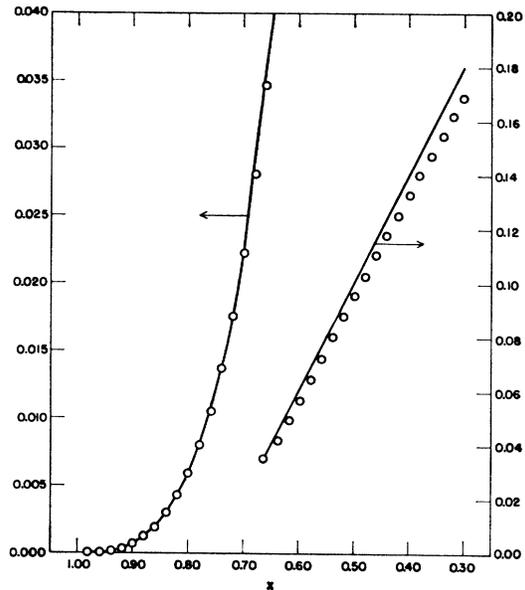
FIG. 2. Relative deformation energy ξ versus fissionability parameter x. Solid lines are the results of this study and marked points (○) are from Ref. 5. For $x \leq 0.66$ the deformation energy is plotted on a $\frac{1}{2}$-scale reduction.

solution of the six simultaneous equations provided the coefficients C_j, and the new estimate of the saddle point was obtained from Eq. (8). This new estimate was used as the initial point in an iterative process with suitable grid size reductions until the following convergence criteria were met:

$$\Delta a = |a_i - a_{SP}| \leq 4.0 \times 10^{-5},$$
$$\Delta b = |b_i - b_{SP}| \leq 4.0 \times 10^{-4}, \quad (9)$$
$$\Delta \xi = |\xi_i - \xi_{SP}| \leq 5.0 \times 10^{-8}.$$

RESULTS AND DISCUSSION

Saddle points were determined for values of x from 0.98 through 0.30 in increments of $\Delta x = 0.02$. Since for $x = 1.00$ the spherical drop is known to be unstable and to have zero deformation energy,[15] no calculations were performed for this value of x.

For each saddle point the following quantities were calculated: the deformation energy ξ, the surface energy B_S, the Coulomb energy B_C, the parallel moment of interia I_{11}, the perpendicular moment of inertia $I_\perp$, the inverse of the effective moment of inertia τ, and the quadrupole moment Q. The parallel moment of inertia I_{11} was taken about the Z axis and the perpendicular moment about an axis at $Z = 0$ perpendicular to the Z axis. The quantity τ is given by $1/I_{11} - 1/I_\perp$. Cohen and Swiatecki's definition[5] of the quadrupole moment was adopted to facilitate comparison with their work.

Table II contains the calculated saddle-point properties. Figures 1 and 2 and Table III are comparisons of

TABLE II. Calculated saddle-point properties and shape parameters of drops defined by Eq. (1) for the range of fissionability parameters.

		Saddle-point properties						Saddle-point parameter values			
x	ξ	B_S	B_C	$I_{\parallel}$	$I_{\perp}$	τ	Q	a	b	c	Z_0
0.98	0.00001	1.00085	0.99957	0.9547	1.0259	0.0728	0.2389	−0.00610	−0.8643	0.9540	1.0466
0.96	0.00005	1.00334	0.99828	0.9117	1.0574	0.1511	0.4880	−0.01933	−0.7380	0.9093	1.0931
0.94	0.00015	1.00740	0.99614	0.8708	1.0949	0.2351	0.7511	−0.03477	−0.6211	0.8656	1.1398
0.92	0.00037	1.01302	0.99312	0.8314	1.1393	0.3251	1.0318	−0.04988	−0.5134	0.8225	1.1871
0.90	0.00072	1.02022	0.98917	0.7934	1.1916	0.4212	1.3346	−0.06341	−0.4142	0.7799	1.2354
0.88	0.00125	1.02903	0.98422	0.7566	1.2533	0.5239	1.6646	−0.07483	−0.3231	0.7374	1.2850
0.86	0.00199	1.03953	0.97818	0.7208	1.3260	0.6333	2.0281	−0.08398	−0.2393	0.6949	1.3361
0.84	0.00301	1.03183	0.97094	0.6859	1.4120	0.7497	2.4332	−0.09093	−0.1622	0.6520	1.3894
0.82	0.00434	1.06608	0.96235	0.6519	1.5144	0.8736	2.8901	−0.09581	−0.0912	0.6084	1.4452
0.80	0.00604	1.08248	0.95222	0.6187	1.6374	1.0054	3.4134	−0.09881	−0.0256	0.5637	1.5042
0.78	0.00818	1.10135	0.94028	0.5865	1.7871	1.1456	4.0235	−0.10011	0.0353	0.5173	1.5673
0.76	0.01085	1.12312	0.92614	0.5551	1.9730	1.2946	4.7513	−0.09987	0.0922	0.4684	1.6357
0.74	0.01413	1.14845	0.90924	0.5250	2.2099	1.4522	5.6460	−0.09822	0.1458	0.4158	1.7115
0.72	0.01815	1.17832	0.88878	0.4969	2.5231	1.6161	6.7898	−0.09526	0.1970	0.3576	1.7973
0.70	0.02309	1.21368	0.86386	0.4730	2.9531	1.7757	8.3111	−0.09122	0.2469	0.2915	1.8962
0.68	0.02908	1.25137	0.83655	0.4594	3.5073	1.8916	10.2135	−0.08742	0.2945	0.2204	1.9998
0.66	0.03605	1.27762	0.81699	0.4610	3.9796	1.9180	11.7911	−0.08675	0.3327	0.1654	2.0690
0.64	0.04359	1.29019	0.80734	0.4692	4.2452	1.8957	12.6536	−0.08886	0.3605	0.1331	2.0971
0.62	0.05140	1.29626	0.80254	0.4784	4.3875	1.8625	13.0098	−0.09211	0.3829	0.1128	2.1056
0.60	0.05936	1.29942	0.79995	0.4872	4.4664	1.8286	13.3345	−0.09584	0.4025	0.0986	2.1052
0.58	0.06739	1.30111	0.79852	0.4956	4.5098	1.7961	13.4517	−0.09979	0.4203	0.0877	2.1003
0.56	0.07547	1.30199	0.79775	0.5035	4.5314	1.7656	13.4976	−0.10388	0.4370	0.0790	2.0931
0.54	0.08357	1.30239	0.79739	0.5109	4.5388	1.7369	13.4974	−0.10805	0.4529	0.0718	2.0844
0.52	0.09167	1.30248	0.79730	0.5180	4.5366	1.7100	13.4663	−0.11229	0.4682	0.0657	2.0749
0.50	0.09978	1.30238	0.79739	0.5248	4.5276	1.6848	13.4135	−0.11657	0.4829	0.0603	2.0650
0.48	0.10788	1.30217	0.79762	0.5312	4.5137	1.6609	13.3453	−0.12089	0.4973	0.0556	2.0548
0.46	0.11597	1.30187	0.79793	0.5374	4.4963	1.6384	13.2664	−0.12523	0.5112	0.0514	2.0446
0.44	0.12404	1.30153	0.79831	0.5434	4.4761	1.6170	13.1788	−0.12963	0.5249	0.0477	2.0342
0.42	0.13210	1.30115	0.79875	0.5491	4.4536	1.5965	13.0841	−0.13409	0.5384	0.0442	2.0238
0.40	0.14014	1.30077	0.79922	0.5547	4.4298	1.5771	12.9858	−0.13855	0.5516	0.0411	2.0136
0.38	0.14816	1.30038	0.79971	0.5601	4.4049	1.5585	12.8841	−0.14306	0.5647	0.0382	2.0034
0.36	0.15617	1.30000	0.80023	0.5653	4.3790	1.5407	12.7800	−0.14760	0.5776	0.0356	1.9934
0.34	0.16415	1.29963	0.80076	0.5703	4.3524	1.5236	12.6738	−0.15220	0.5903	0.0331	1.9834
0.32	0.17210	1.29927	0.80131	0.5753	4.3254	1.5072	12.5667	−0.15682	0.6029	0.0308	1.9736
0.30	0.18004	1.29892	0.80166	0.5800	4.2979	1.4913	12.4587	−0.16150	0.6154	0.0287	1.9639

data calculated in this study with those of Cohen and Swiatecki.[5] In Fig. 1 cross sections of the deformation-energy saddle-point drop shapes are illustrated, while in Fig. 2 the deformation energy ξ is plotted versus the fissionability parameter x for a few values in the range of x. Table III consists of the percent difference between the calculated saddle point properties and those of Ref. 5 for a few values of x.

From Table III it is seen that all of the calculated properties are within 5% of Cohen and Swiatecki's properties[5] for $x \geq 0.70$. In support of this result, Fig. 1 also indicates a close agreement in drop shapes for this range of x. This is consistent with Cohen and Swiatecki's result[5] that only the first two of their parameters had appreciable magnitude for the same x range.

As yet no study of the dynamical motions of the

TABLE III. Percent difference between saddle point properties calculated in this two-parameter study and those properties calculated by Cohen and Swiatecki (see Ref. 5), using nine parameters. The superscript CS refers to Ref. 5.

x	$\delta\xi/\xi^{CS}$	$\delta B_S/B_S^{CS}$	$\delta B_C/B_C^{CS}$	$\delta I_{\parallel}/I_{\parallel}^{CS}$	$\delta I_{\perp}/I_{\perp}^{CS}$	$\delta\tau/\tau^{CS}$	$\delta Q/Q^{CS}$
0.90	+1.41%	+0.03%	−0.02%	−0.19%	+0.17%	+0.86%	+0.85%
0.80	+2.20%	+0.23%	−0.15%	−0.85%	+1.18%	+2.11%	+2.45%
0.70	+3.26%	+0.67%	−0.61%	−1.87%	+3.64%	+3.00%	+4.77%
0.60	+4.23%	+1.08%	−1.18%	−0.75%	+7.01%	+1.72%	+8.05%
0.50	+4.65%	+1.24%	−1.42%	+0.46%	+8.76%	+0.55%	+9.94%
0.40	+5.50%	+1.60%	−2.30%	+1.08%	+10.76%	+0.70%	+15.32%
0.30	+6.38%	+1.71%	−2.24%	+2.53%	+20.06%	−0.65%	+16.89%

liquid drop has been made with precision comparable to the static investigations of Cohen and Swiatecki.[5] Both Kelson's and Nix's simplified dynamical treatments[9,10] provide static saddle-point properties which agree best with Cohen and Swiatecki's[5] for elements less massive than radium (fissionability parameter $\simeq 0.70$). It is hoped that the present investigations will provide a few-parameter basis for dynamical calculations of adequate precision, even for x values approaching 1.00. Studies directed towards this goal are presently under way.

Inelastic Scattering and Neutron Pickup for ^{12}C and ^{16}O Projectiles on ^{208}Pb*†

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^{208}Pb nuclei have been bombarded with ^{12}C and ^{16}O projectiles under conditions where a semiclassical description of the process should be valid. In the bombardment of ^{208}Pb with 126.5-MeV ^{12}C ($\eta = ZZ'e^2/\hbar v = 24.5$), two inelastic-scattering peaks are observed corresponding to $Q = -2.7\pm0.3$ MeV and -4.5 ± 0.3 MeV. The angular distributions of the inelastically scattered ^{12}C show a monotonic increase with decreasing angle until a maximum is reached at about $\theta_{c.m.} = 35°$. This angle corresponds to grazing collisions, assuming that particles follow Rutherford trajectories. The $Q = -2.7$-MeV peak is identified as the excitation of the 2.6-MeV state in ^{208}Pb. The $Q = -4.5$-MeV peak could be the excitation of the 4.4-MeV state in ^{12}C or the 4.3-MeV state in ^{208}Pb. The inelastic scattering cross section for the excitation of the 2.6-MeV ^{208}Pb state by ^{16}O projectiles having approximately the same velocity (166.4 MeV) is a factor of 2 smaller than when ^{12}C is used as a projectile; this result is somewhat surprising since the semiclassical conditions are similar and the elastic-scattering cross sections differ only by 20%. The cross section for the 4.5-MeV excitation is not observed and is smaller by more than a factor of 4. Therefore, in the ^{12}C+^{208}Pb case, the major contribution to the 4.5-MeV excitation very likely originates from the excitation of the 4.4-MeV state in ^{12}C. The reactions ^{208}Pb(^{16}O, ^{17}O)^{207}Pb and ^{208}Pb(^{12}C, ^{13}C)^{207}Pb were also observed in these experiments. Both angular distributions have a maximum differential cross section of 100 mb/sr, which is considerably larger than those ordinarily observed in neutron-transfer reactions. The excitation energies are consistent in both reactions with neutrons being picked up by the projectiles into $d_{5/2}$ states.

I. INTRODUCTION AND SUMMARY

IN recent years, it has been found that in inelastic scattering, the collective levels are more strongly excited than others, regardless of the projectiles used. The preferential excitation of collective levels by alpha particles has been pointed out by Blair.[1] Cohen[2] has noted the similarity between the inelastic scattering of protons and deuterons and has emphasized the collective nature of the process. High-energy electron scattering[3] has been shown to strongly excite levels known to be collective. Heavy-ion (^{12}C) inelastic scattering has also been shown [4,5] to be very similar to the alpha-particle scattering. This enhancement can be understood in terms of the similarity between the matrix elements of inelastic scattering and electric transitions, as pointed out by Pinkston and Satchler.[6] Therefore regardless of the projectiles used, the inelastic-scattering process has proved to be a good method for investigating collective states.

In the heavy-ion studies of inelastic scattering, the

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