Electrostatic potentials for nucleus-nucleus optical model

A. K. Jain, M. C. Gupta, and C. S. Shastry
Department of Physics, Birla Institute of Technology and Science, Pilani-333031, India
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The electrostatic potential between nuclei having arbitrary charge distributions is expressed as a triple integral. For two nuclei having uniform distributions, an algebraic expression for the electrostatic potential is obtained. This is then compared with the electrostatic potentials normally used in various nucleus-nucleus optical model calculations. The results of the former are found to be significantly different from the latter. For Fermi-Fermi types of charge distributions, the nuclei may be assumed to be uniformly charged spheres without much loss of accuracy. If one of the charge distributions has either Gaussian or harmonic well shape, the triple integral is reduced to a single integral. For a number of nucleus-nucleus pairs, we have calculated the electrostatic potentials assuming them to be uniformly charged spheres and compared them with those derived from realistic charge distributions. With a proper choice of radius parameters, the former can be used to a good degree of accuracy to generate the electrostatic potential between the nuclei.

[NUCLEAR REACTIONS Realistic Coulomb potential for optical model.]

I. INTRODUCTION

In the proton-nucleus optical model of elastic scattering, it is customary to use the electrostatic potential (ESP) derived by assuming the proton as a point charge and the nucleus as a uniformly charged sphere.[1-3] However, it is known that the realistic charge distributions of various nuclei differ considerably from the uniform distribution. For light nuclei like ^{7}Li, ^{12}C, ^{16}O, etc., charge densities vary like a Gaussian function or harmonic well, and in heavy nuclei like ^{40}Ca it is close to a Fermi distribution.[4] There have been calculations estimating the deviations of the ESP between proton and nucleus due to realistic charge distribution as compared with the uniform one.[5] It is found that the difference is usually about 5–8%. In the case of nucleus-nucleus scattering however, a concrete estimate of the ESP has not been made and many of the nucleus scattering calculations use the ESP between a suitably chosen uniformly charged sphere and a point charge.

In Sec. II we derive the expression for the ESP between two nuclei with arbitrary charge distributions. An algebraic expression for uniform charge distributions is obtained so that it is readily applicable in any nucleus-nucleus scattering calculations. In Sec. III we compare numerically the expression for the ESP between uniformly charged spheres obtained by us with the normally used expressions. The results with realistic charge distributions are also compared with those obtained with uniform charge distributions for various combinations of nuclei having different functional forms for the charge distribution. Section IV gives the summary and the conclusions.

II. ELECTROSTATIC POTENTIAL BETWEEN TWO NUCLEI HAVING ARBITRARY CHARGE DISTRIBUTIONS

Let $\rho_1(r)$ and $\rho_2(r)$ be the spherically symmetric charge distributions corresponding to the two nuclei A and B with their centers a distance R apart. The ESP between A and B is then

$$V(R) = \int\int \frac{\rho_1(r_1)\rho_2(r')}{|\vec{r}_1 - \vec{r}_2|}\, d\vec{r}_1 d\vec{r}_2 , \tag{2.1}$$

where $\vec{r}_1$, $\vec{r}'$, and $\vec{r}_2$ are as shown in Fig. 1 and $r' = (r_2^2 + R^2 - 2r_2Rz)^{1/2}$ where $z = \cos\theta$. Using the expansion

$$\frac{1}{|\vec{r}_1 - \vec{r}_2|} = \frac{4}{r_>} \sum_{l,m} \left(\frac{r_<}{r_>}\right)^l \frac{1}{(2l+1)}\, Y_{lm}(\hat{r}_1) Y^*_{lm}(\hat{r}_2),$$

where $r_< = r_1$, $r_> = r_2$ for $r_1 \leq r_2$ and $r_< = r_2$, $r_> = r_1$ for $r_1 \geq r_2$. Carrying integration over angular coordinates of $\vec{r}_1$ we obtain

$$V(R) = 8\pi^2 \int_0^\infty \rho_1(r_1) r_1^2 dr_1 \int_0^\infty \frac{r_2^2 dr_2}{r_>} \times \int_{-1}^{1} \rho_2(r_2^2 + R^2 - 2r_2Rz)^{1/2} dz . \tag{2.2}$$

In the case of uniformly charged nuclei with radii a_1 and $a_2 (a_2 \geq a_1)$ and charge numbers Z_1 and Z_2 the triple integration in Eq. (2.2) can be easily

performed to get

$$V(R) = Z_1 Z_2 e^2/R, \quad R \geq (a_1 + a_2)$$

$$= \frac{3Z_1Z_2e^2}{8a_1^3a_2^3R}\left(\tfrac{1}{12}(a_1^6 + a_2^6) - \tfrac{3}{4}(a_1^2a_2^4 + a_2^2a_1^4) + \tfrac{4}{3}a_1^3a_2^3 + 2R[(a_1^3a_2^2 + a_1^2a_2^3) - \tfrac{1}{5}(a_1^5 + a_2^5)]\right.$$

$$\left. + \frac{3R^2}{4}(a_1^2 - a_2^2)^2 - \frac{2R^3}{3}(a_1^3 + a_2^3) + \tfrac{1}{4}R^4(a_1^2 + a_2^2) - \frac{R^6}{60}\right), \quad (a_1 + a_2) \geq R \geq (a_2 - a_1)$$

$$= \frac{3Z_1Z_2e^2}{2a_1^3a_2^3}[(a_1^3a_2^2 - \tfrac{1}{5}a_1^5) - \tfrac{1}{3}(R^2a_1^3)], \quad (a_2 - a_1) \geq R \geq 0. \tag{2.3}$$

If $\rho_2(r)$ has a Gaussian form

$$\rho_2(r) = \rho_0 e^{-r^2/\alpha^2}, \quad \rho_0 = Ze/(\pi^{3/2}\alpha^3)$$

or a harmonic well form

$$\rho_2(r) = \rho_0\left(1 + \frac{\omega}{\alpha^2}r\right)e^{-r^2/\alpha^2}, \quad \rho_0 = \frac{Ze}{\pi^{3/2}\alpha^3(1 + \frac{3}{2}\omega)}$$

the integration over r_2 and z can be performed analytically. The result as a function of r_1 is given by

$$I(r_1) = W(X_1 + X_2 + X_3), \quad r_1 \leq R$$
$$= W[X_1 + X_2 - (r_1 + R)X_4 + \alpha X_5], \quad r_1 \geq R. \tag{2.4}$$

For Gaussian form the quantities appearing in Eq. (2.4) are given by

$$W = Ze/(4R\pi^{3/2}),$$
$$X_1 = \alpha(e^{-\xi} - e^{-\eta}), \quad \xi = (r_1 + R)^2/\alpha^2, \quad \eta = (r_1 - R)^2/\alpha^2,$$
$$X_2 = (r_1 + R)\gamma(\tfrac{1}{2}, \xi), \quad X_3 = (r_1 - R)\gamma(\tfrac{1}{2}, \eta), \tag{2.5}$$
$$X_4 = \gamma(\tfrac{1}{2}, \zeta), \quad \zeta = 4R^2/\alpha^2,$$
$$X_5 = 1 - e^{-\zeta}.$$

$\gamma(x, y)$ are incomplete γ functions. For harmonic well form

$$W = Ze/[4R\pi^{3/2}(1 + \tfrac{3}{2}\omega)],$$
$$X_1 = \alpha[1 + \omega(2 + \xi)]e^{-\xi} - \alpha[1 + \omega(2 + \eta)]e^{-\eta},$$
$$X_2 = (r_1 + R)[(1 + \omega)\gamma(\tfrac{1}{2}, \xi) + \omega\gamma(\tfrac{3}{2}, \xi)],$$
$$X_3 = (r_1 - R)[(1 + \omega)\gamma(\tfrac{1}{2}, \eta) + \omega\gamma(\tfrac{3}{2}, \eta)], \tag{2.6}$$
$$X_4 = (1 + \omega)\gamma(\tfrac{1}{2}, \zeta) + \omega\gamma(\tfrac{3}{2}, \zeta),$$
$$X_5 = (1 + 2\omega)(1 - e^{-\zeta}) - \omega\zeta e^{-\zeta}.$$

Thus, if either of the two nuclei has either the Gaussian or the harmonic well type charge distribution, then the triple integral in Eq. (2.2) reduces to a single integral which may readily be performed numerically. In the next section we compare

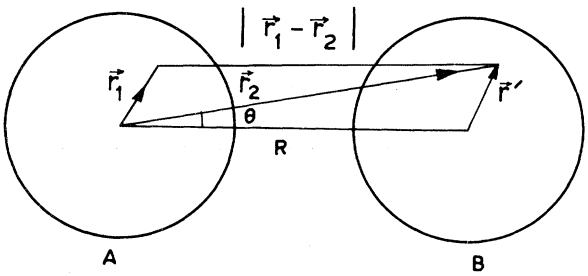

FIG. 1. Two spherically symmetric charge distributions, A and B with their centers a distance R apart, showing the various quantities in Eq. (2.1).

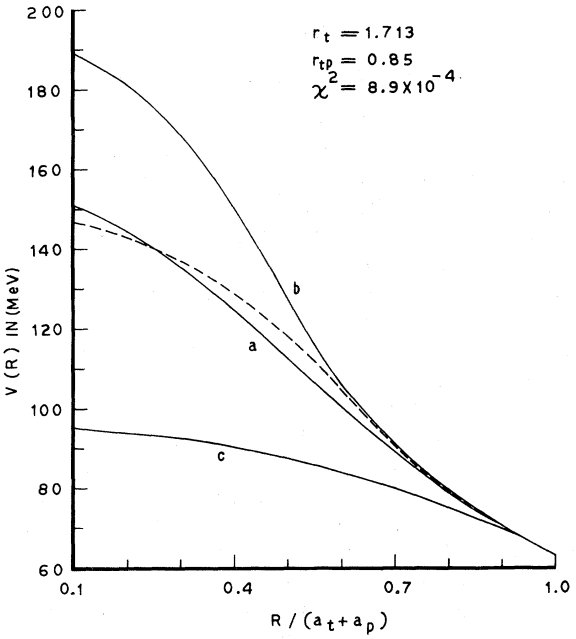

FIG. 2. Electrostatic potentials obtained from Eq. (2.3) (curve a) and Eq. (3.1) with $R_c = a_t$ (curve b) and $R_c = (a_t + a_p)$ (curve c) for the ^{40}Ca–^{40}Ca system. The results with minimum χ^2 given by Eq. (3.2) are shown as a dashed line.

TABLE I. The charge distribution parameters for various nuclei. All lengths are expressed in fm.

Nucleus	Type of charge distribution	Radius parameter	Skin thickness	Half-density radius	Radius of equivalent uniform model
^{6}Li	Gaussian $\alpha=\frac{1}{3}$	1.56	...	...	2.84
^{7}Li	Gaussian $\alpha=\frac{1}{3}$	1.49	...	...	2.84
^{16}O	Harmonic well $\omega=2.0$, $\alpha=1.75$	1.35	1.9	2.6	3.41
^{40}Ca	Fermi	1.32	2.5	3.64	4.54
^{197}Au	Fermi	1.18	2.32	6.38	6.87

the ESP between two uniformly charged spheres with that obtained by assuming one of them as point charge. Then we compare the results with realistic and uniform distributions.

III. COMPARISON OF ELECTROSTATIC POTENTIALS FROM VARIOUS CHARGE DISTRIBUTIONS

If one assumes the nuclei to be uniformly charged spheres, Eq. (2.3) provides a simple algebraic expression for the ESP for use in the nucleus-nucleus optical model calculations. However, in such calculations the expression used is the ESP between a point charge and a uniformly charged sphere and is

$$V(R) = Z_1 Z_2 e^2/R, \quad R \geq R_c$$
$$= Z_1 Z_2 e^2(3R_c^2 - R^2)/(2R_c^3), \quad R \leq R_c, \quad (3.1)$$

where R_c is chosen[1,6] to be either $r_t A_t^{1/3}$ or $r_{tp}(A_t^{1/3} + A_p^{1/3})$ where r_t and r_{tp} are adjustable parameters and A_t and A_p are the mass numbers of the target and the projectile, respectively. We now examine the validity of these two models compared to $V(R)$ given by Eq. (2.3). We do this for two types of combinations—(i) when the two nuclei are of comparable sizes and (ii) when one of them is large compared to the other. Figure 2 shows the results of calculations from Eq. (2.3) (curve a) and Eq. (3.1) for the ^{40}Ca-^{40}Ca system. The radii a_t and a_p of the nuclei were calculated from radius parameters given in Ref. 4 and are tabulated in Table I. It is seen that for the separation where R is small compared to $(a_t + a_p)$, the results with either $R_c = a_t$ (curve b) or $R_c = (a_t + a_p)$ (curve c) differ considerably from curve a. They however become very close to it for $R \simeq (a_t + a_p)$. Parameters r_t and r_{tp} were varied to get the minimum value of χ^2 defined by

$$\chi^2 = \frac{\sum_i [V_1(R_i) - V_2(R_i)]^2}{\sum_i [V_2(R_i)]^2}, \quad (3.2)$$

where $V_1(R_i)$ and $V_2(R_i)$ are the ESP's given by Eqs. (3.1) and (2.3), respectively. A total of 20 points were taken from $0.05(a_t + a_p)$ to $(a_t + a_p)$. The results with either $R_c = r_t A_t^{1/3}$ or $R_c = r_{tp}(A_t^{1/3} + A_p^{1/3})$ are practically the same and are shown as a dashed curve in Fig. 2. The values of r_t and r_{tp} are found to be 1.713 and 0.85, respectively. Figure 3 shows similar calculations for the ^{7}Li-^{197}Au system. Here the results are comparatively better because one of the nuclei is very small compared to the other and can be treated as a point charge. The parameters r_t and r_{tp} for minimum χ^2 (calculated in the same way as for

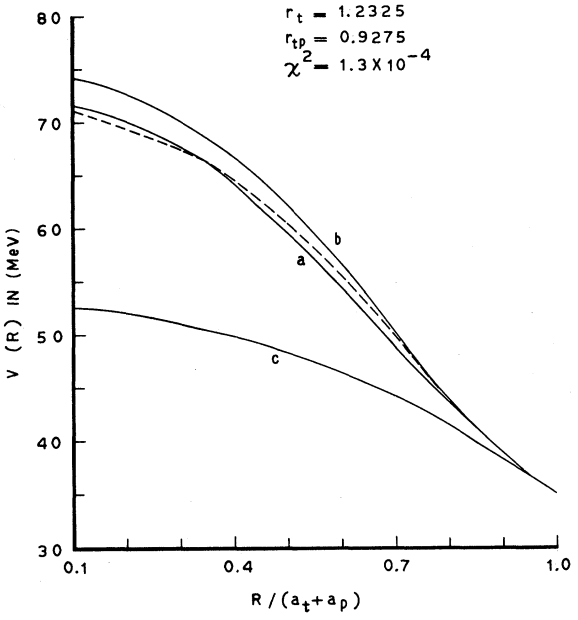

FIG. 3. Electrostatic potentials obtained from Eq. (2.3) (curve a) and Eq. (3.1) with $R_c = a_t$ (curve b) and $R_c = (a_t + a_p)$ (curve c) for the ^{7}Li–^{197}Au system. The results with minimum χ^2 given by Eq. (3.2) are shown as a dashed line.

Fig. 2) are found to be 1.2325 and 0.9275, respectively. The radius parameters of the nuclei are taken from Ref. 4 and are given in Table I. It should be noted that the parameters r_t or r_{tp} corresponding to the best χ^2 in our case are quite different from the parameters used in the nucleus-nucleus optical model calculations.[6] This shows that the ESP is not correctly reproduced in general in nucleus-nucleus optical model calculations.

It should however be stressed that for many nuclei the assumption of uniform charge distribution is a poor one. This is particularly so for light nuclei like ^{6}Li, ^{12}C, and ^{16}O where the charge distribution is either of the Gaussian or harmonic well type.[4] Therefore, it is important to consider the exact ESP given by Eq. (2.2) and to examine to what extent Eq. (2.3) is a good approximation to it. In the case of heavy nuclei like ^{40}Ca, ^{197}Au, etc. the charge distribution is of the Fermi type for which uniform distribution is a reasonably good approximation and the potentials given by Eqs. (2.3) and (2.2) can be expected to have good agreement.

Figures 4 and 5 give the results of calculations for a variety of combinations of nuclei having different types of charge distributions. The solid curves show the results obtained from Eq. (2.2) with realistic charge distributions and the dashed curves show the results from Eq. (2.3). As expected for the ^{40}Ca-^{40}Ca system, the two results agree fairly well at all separations between the nuclei. But for other combinations, the two results differ substantially at small separations. To get a good fit with exact results the radii of the nuclei were put as $a_p' = r_0' A_p^{1/3}$ and $a_t' = r_0'' A_t^{1/3}$ and the parameters r_0' and r_0'' are varied to get minimum values of χ^2 defined in Eq. (3.2), where V_1 and V_2 are now given by Eqs. (2.3) and (2.2), respectively. Thirty points were taken from $0.1(a_t + a_p)$ to $3(a_t + a_p)$ to evaluate χ^2. The values of r_0', r_0'', and χ^2 for least χ^2 are also mentioned along with the curves. The various charge distribution parameters are tabulated in Table I. From these figures one finds that with the proper choice of appropriate parameters, the algebraic expression Eq. (2.3) reproduces the ESP obtained with realistic charge distributions quite well at large separations between the nuclei, and the agreement in most cases is qualitative when the separation is smaller. For the Fermi-Fermi type of combination, no change in radius parameters is necessary in view of the good agreement between the Eqs. (2.2) and (2.3). In the next section we present the conclusions based on the analysis carried out in Secs. II and III.

IV. DISCUSSION AND CONCLUSIONS

From the analysis carried out in earlier sections we can draw the following conclusions. It is

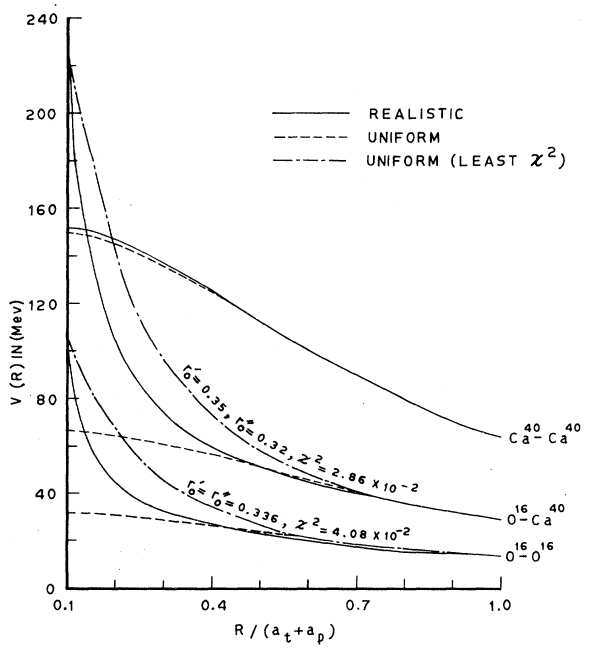

FIG. 4. Electrostatic potentials assuming realistic and uniform charge distributions for ^{40}Ca–^{40}Ca, ^{16}O–^{16}O, and ^{16}O–^{40}Ca systems. The curves with minimum χ^2 defined in Eq. (3.2) are shown as dash-dotted lines.

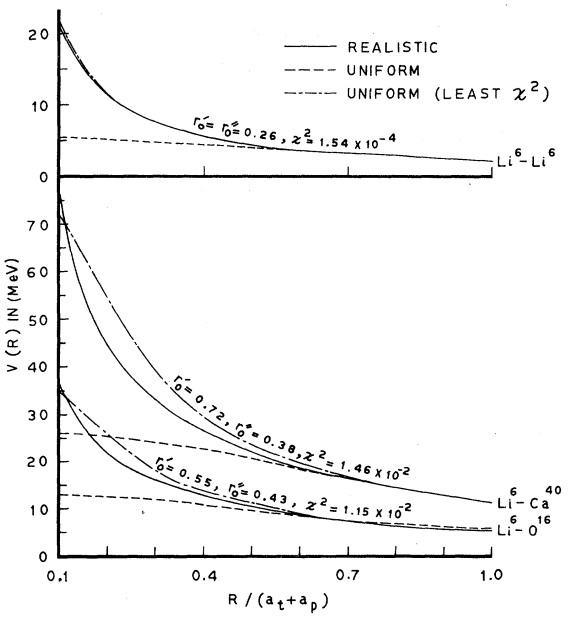

FIG. 5. Electrostatic potentials assuming realistic and uniform charge distributions for ^{6}Li–^{6}Li, ^{6}Li–^{40}Ca, and ^{6}Li–^{16}O systems. The curves with minimum χ^2 defined in Eq. (3.2) are shown as dash-dotted lines.

found that there is a significant amount of error involved in ESP when one approximates one of the nuclei as a point charge, compared to the case of two uniformly charged finite spheres. The error may be as high as 25% at small separations between two nuclei of comparable sizes, such as the ^{40}Ca-^{40}Ca system, when we put $R_c = a_t$ in Eq. (3.1). The error is much more if $R_c = (a_t + a_p)$ is taken and the two results may even differ by a factor of 2 for $R < 0.1R_c$. Similar conclusions were recently reported by DeVries.[7] When the size of one of the nuclei is very small compared to the other, the error with $R_c = a_t$ is comparatively small because the smaller nucleus may be taken as a point charge. In both the cases, a parameter (r_t or r_{tp}) may be varied to get a minimum χ^2 fit. But, as pointed out earlier, the order of values obtained for radius parameters r_t or r_{tp} are much different from those used in optical model calculations.[6] The exact expressions for the Coulomb potential given by Eq. (2.3) should therefore be used if the nuclei are assumed to be uniformly charged spheres.

The realistic charge distribution is however far from uniform, especially for light nuclei like ^{6}Li, ^{12}C, ^{16}O, etc. Calculations with the actual charge distributions show that the ESP between two nuclei is not properly reproduced at small separations if the nuclei are assumed to be uniformly charged spheres. The height of the Coulomb barrier is much more enhanced if realistic charge distribution is taken. This is clear from Figs. 4 and 5. Here also one can vary two parameters r_0' and r_0'' to get the minimum χ^2 fit, but good fit is still not obtained except for the ^{6}Li-^{6}Li system. The reason for getting a good fit in this case is that the charge density in ^{6}Li falls off too fast (see Table I). In the case of heavy nuclei such as ^{40}Ca, ^{197}Au, etc., the charge distribution is of the Fermi type, which is very close to the uniform distribution. Thus when both the nuclei have a Fermi type charge distribution, the algebraic expression in Eq. (2.3) is sufficiently accurate and convenient to be incorporated in optical model calculations. But for other types of distributions one has to solve the triple integral in Eq. (2.2). In case one of the nuclei has a Gaussian or harmonic well type distribution, r_2 and z integrations in Eq. (2.2) can be performed analytically and are given by Eqs. (2.4)–(2.6). Thus for all combinations other than the Fermi-Fermi, the expression for $V(R)$ is in terms of a single integral and for the Fermi-Fermi combination, the algebraic expressions in Eq. (2.3) are reasonably good. So in no case is a numerical computation of the triple integral required and Eq. (2.2) can be used economically in any nucleus-nucleus optical model calculation. The computation time can further be reduced if we note from Figs. 4 and 5 that after a distance of about $\frac{1}{2}(a_t + a_p)$ the uniform charge distribution gives fairly good results. Thus while calculating the electrostatic potential, one may perform numerical integration only up to a certain distance, say $\frac{1}{2}(a_t + a_p)$ and after that the algebraic expressions in Eq. (2.3) can be used. The nucleus-nucleus optical model calculations using the electrostatic potentials stated in this paper will be described in a future publication.

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