Truncated Matching Potentials in the Classical Theory of Elastic Atomic Scattering

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Atomic collisions in the radiation damage of solids can be described by repulsive potentials for which the scattering integrals cannot generally be evaluated in closed form. However, the evaluation becomes possible when the actual interatomic potential is replaced by certain truncated power potentials which match the actual potential in value and in slope at the minimum distance. The usefulness and accuracy of such matching potentials are discussed and numerical examples are given for the scattering angle, the "time integral," and the energy transfer in the cases of an exponential potential and of an exponentially screened Coulomb potential. The agreement with the exact numerical solutions is surprisingly good.

I. INTRODUCTION

A DETAILED analysis of the slowing down of energetic atoms in solids is fundamental to the theory of radiation damage and sputtering. If the energy of the atoms is not too great, its slowing down may be attributed to its elastic encounters with the atoms of the solid, energy losses by electron excitation being ignored. If the energy of the moving particle is not too small, its interactions with the target particles may be regarded as isolated from each other and the classical theory of scattering from a conservative, central, purely repulsive potential may be applied. The conditions for the applicability of classical mechanics have been discussed before.[1,2] For most applications in the intermediate energy region, it is sufficient to evaluate the asymptotic properties of the particle trajectories. In fact, the validity of the two-body treatment of atomic slowing down problems in solids depends in a general way on the actual particle trajectories adhering rather closely to their asymptotes. Unfortunately, the classical scattering integrals can be evaluated in closed form in terms of standard tabulated functions only for a limited group of power potentials.[3] For the potentials of primary interest in radiation damage theory, it is necessary to use approximation methods or to evaluate the integrals numerically. It is the purpose of this commmunication to investigate the accuracy of some of the approximate treatments of the scattering integrals which have been proposed for radiation damage applications. This will be accomplished by the systematic discussion of a class of matching potentials, using in part a perturbation expansion, and by the direct numerical comparison of the approximate solutions with recently published tables of exact values.[4]

Consider, as in Fig. 1, a moving atom, the projectile, of mass m_1 and initial laboratory (L) kinetic energy E, to be scattered by an initially stationary atom, the target, of mass m_2. The location of the asymptotic trajectories of the two particles in the L system can be given in terms of the center-of-mass (c.m.) scattering angle θ and the "time integral" τ which describes the location of the c.m. when the distance between the two particles is a minimum. The two scattering integrals are[3]

$$\theta=\pi-2s\int_R^\infty dr[r^2f(r)]^{-1}, \tag{1}$$

$$\tau=(R^2-s^2)^{1/2}-\int_R^\infty dr\{[f(r)]^{-1}-[1-s^2/r^2]^{-1/2}\}, \tag{2}$$

where

$$f(r)=[1-s^2/r^2-\phi(r)/E_r]^{1/2}, \tag{3}$$

$E_r=AE/(1+A)$, and $A=m_2/m_1$; s is the impact parameter, r is the (variable) interatomic separation, $\phi(r)$ is the potential of interaction, and R is the distance of closest approach, defined by $f(R)=0$. Figure 1 shows the L coordinates of the two particles and of their c.m. when $r=R$. Note that in conventional scattering

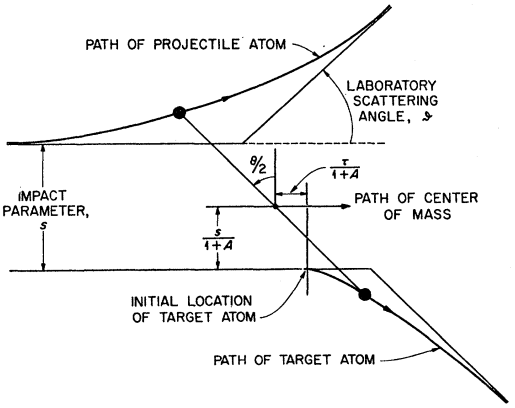

FIG. 1. Trajectories of the particles in a two-body collision. The positions of the particles are shown at their minimum separation.

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[2] C. Lehmann and G. Leibfried, Z. Physik **172**, 465 (1963).

[3] H. Goldstein, *Classical Mechanics* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1956), pp. 58–92.

[4] M. T. Robinson, *Tables of Classical Scattering Integrals for the Bohr, Born-Mayer, and Thomas-Fermi Potentials*, U. S. Atomic Energy Commission. Report ORNL-3493, 1963 (unpublished). (Available from Office of Technical Services, Department of Commerce, Washington 25, D. C.)

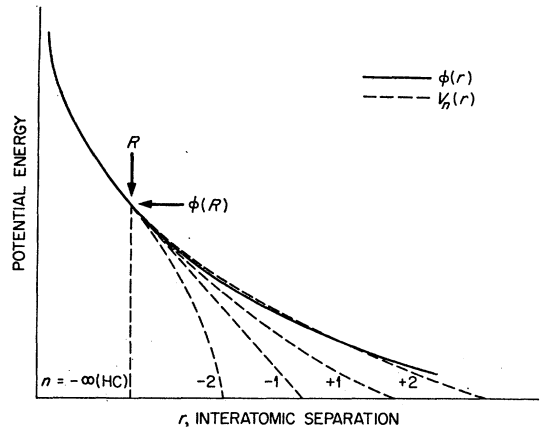

FIG. 2. An actual potential, $\phi(r)$, matched by a series of truncated power potentials, $V_n(r)$.

theory,[3] where the detector of the scattered particle is regarded as very far from the scattering center, the "time integral" may be neglected, but that this cannot be done in discussing multiple scattering problems in solids, for now the "detector" is the next scattering center and is only distant by an amount of the same order as s and τ.

Under circumstances where θ is small, that is, for E_r or s large, the integrals (1) and (2) may be treated with sufficient accuracy by the momentum (impulse) approximation (MA).[1,2,5] The exact interatomic potential $\phi(r)$ is regarded as a perturbation and the integrals are evaluated from this viewpoint. A detailed discussion of the MA has been given by Lehmann and Leibfried.[2] On the other hand, when θ is not small, the exact potential may be replaced by an approximate one for which the scattering integrals may be evaluated in terms of tabulated functions. We shall discuss a family of such approximations which includes as special cases the well-known hard-core approximations,[6-8] the energy-independent matching potentials,[1,9] and various more elaborate matching potential procedures.[8,10,11] The approach is essentially an elaboration of the work of Leibfried and Oen[11] and includes their results as a special case. While several useful remarks about the accuracy of the various approximations will be made, the most convenient test of their value is based on comparison with exact numerical solutions of Eqs. (1) and (2).

II. GENERAL DISCUSSION OF THE MATCHING POTENTIALS

Since our discussion has been restricted to purely repulsive potentials, it is required that

$$\phi(r)\geqslant 0 \quad \text{and} \quad \phi'(r)\leqslant 0 \quad 0<r<\infty \tag{4}$$

where the prime means d/dr. Furthermore, in order that the integral in Eq. (2) be defined, it is necessary that $\lim_{r\to\infty} r\phi(r)=0$. No other general restrictions of $\phi(r)$ will be made. The potential $\phi(r)$ will be approximated by matching to it the family of truncated power potentials

$$\begin{aligned} V_n(r)&=(\alpha_n/n)[(\beta_n/r)^n-1], && 0<r<\beta_n,\\ &=0, && \beta_n<r<\infty, \end{aligned} \tag{5}$$

where α_n and β_n are constants and where the index n can take on any value, positive or negative. The difference between the exact and approximate potentials is

$$\Delta_n(r)=\phi(r)-V_n(r)\,. \tag{6}$$

The parameters α_n and β_n will be evaluated by matching $V_n(r)$ to $\phi(r)$ in value and in slope at the point of minimum separation of the two interacting particles; that is, it is required that

$$\Delta_n(R)=\Delta_n'(R)=0, \tag{7}$$

from which follow immediately

$$\alpha_n=-[n\phi(R)+R\phi'(R)]=-g_n'(R)/R^{n-1}, \tag{8}$$

$$\beta_n=R[-R\phi'(R)/\alpha_n]^{1/n}, \tag{9}$$

where

$$g_n(r)=r^n\phi(r)\,. \tag{10}$$

It is evident that for $V_n(r)$ to be a *plausible* approximation to $\phi(r)$, it must be positive and must obey $\lim_{r\to\infty} rV_n(r)=0$, which requires $\alpha_n>0$ and $\beta_n>0$. Hence, in addition to the restrictions (4), it is necessary that

$$n\phi(R)<-R\phi'(R) \quad \text{or} \quad g_n'(R)<0 \tag{11}$$

from which it can be seen that, for any R, there is a maximum value of n corresponding to a plausible approximation. At $n_{\max}$, β_n becomes infinite and the approximation corresponds to one suggested by Holmes *et al.*[10] Inserting Eqs. (8) and (9) into (5),

$$V_n(r)=\phi(R)+[R\phi'(R)/n][1-(R/r)^n] \quad 0<r<\beta_n, \tag{12}$$

Two limiting cases of Eq. (12) may be mentioned:

$$V_0(r)=\phi(R)+R\phi'(R)\ln(r/R) \quad 0<r<\beta_0,$$

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[9] K. O. Nielsen, in *Electromagnetically Enriched Isotopes and Mass Spectrometry* (Academic Press Inc., New York, 1956), p. 68; J. Lindhard, V. Nielsen, N. Scharff, and P. V. Thomsen, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **33**, No. 10 (1963).
[10] D. K. Holmes, G. Leibfried, and O. S. Oen, Solid State Division Annual Progress Report, 1959, U. S. Atomic Energy Commission Report ORNL-2829 (unpublished). (Availability as in Ref. 4.)
[11] G. Leibfried and O. S. Oen, J. Appl. Phys. **33**, 2257 (1962).

where $\beta_0=R\exp[-\phi(R)/R\phi'(R)]$ and

$$V_{-\infty}(r)=V_{\mathrm{HC}}(r)=\phi(R)\,,\quad 0<r<R,\qquad =0\,,\quad R<r<\infty\,, \tag{13}$$

which is the potential corresponding to scattering from an impenetrable sphere. Thus, the well-known hard-core (HC) approximation[6–8] is included in the family $V_n(r)$, although in a somewhat different guise than usual. Figure 2 illustrates schematically a family of approximations matched to an actual potential in the manner specified in Eq. (7). Note that this matching scheme produces parameters which are (generally) functions of both energy and impact parameter.

It follows from Eq. (12) that

$$\partial V_n(r)/\partial n\gtrless 0\,, \tag{14}$$

which expresses the order of the approximate potentials with respect to each other. If $\phi(r)$ is replaced in Eqs. (1) and (2) by $V_n(r)$, no change occurs in the lower limit of the integrals, on account of the matching in Eq. (7). Hence, denoting the approximate values of θ and τ by $\theta_{\mathrm{app}}(n)$ and $\tau_{\mathrm{app}}(n)$, it follows from Eqs. (1) and (2) and the inequality (14) that

$$\partial\theta_{\mathrm{app}}(n)/\partial n\lessgtr 0\quad\text{and}\quad\partial\tau_{\mathrm{app}}(n)/\partial n\lessgtr 0 \tag{15}$$

which express the order of the approximations with respect to each other. The positions of the exact values in the sequences (15) depend upon whether or not $\Delta_n(r)$ is ever negative, a question which is examined in Appendix A. If $\Delta_k(r)>0$, then $\theta_{\mathrm{app}}(k)>\theta$ and all $n<k$ correspond to approximations of less accuracy than this one. If k can be chosen so that $g_k(r)$ [Eq. (10)], always obeys $g_k'(r)<0$ and $g_k''(r)>0$, then $\Delta_k(r)>0$ whatever the values of r and R. These conditions are sufficient, but, for $k>1$, the second one is not actually necessary so that caution in applying these remarks is warranted.

The accuracy of the $V_n(r)$ as approximating potentials for scattering problems may be investigated in more detail by regarding $\Delta_n(r)$ as a perturbation, in a manner reminescent of that used by Lehmann and Leibfried in their discussion of the MA.[2] The treatment here is much simpler, since the limits of the integrals in Eqs. (1) and (2) are not changed when $V_n(r)$ replaces $\phi(r)$: Methods of complex integration are not required and the restriction that $\phi(r)$ be a regular function is unnecessary. The perturbation treatment of θ is outlined here; that for τ is exactly similar and will be omitted. First, replace $\phi(r)$ in Eq. (1) by $V_n(r)+\Delta_n(r)$. Then, define

$$f_n(r)=[1-s^2/r^2-V_n(r)/E_r]^{1/2} \tag{16}$$

$$h_n(r)=\Delta_n(r)/E_r[f_n(r)]^2. \tag{17}$$

As long as $|h_n(r)|<1$ for $R<r<\infty$, $f(r)$ in the integrand of Eq. (1) can be expanded and then

$$\theta=\pi-\sum_{k=0}^{\infty}\theta_k(n)\,, \tag{18}$$

with

$$\theta_k(n)=2s\gamma_k\int_R^{\infty}dr[h_n(r)]^k[r^2f_n(r)]^{-1}, \tag{19}$$

where

$$\gamma_k=(2k)!/2^{2k}(k!)^2.$$

That the condition for the convergence of the sum (18) is the same as for the expansion of $f(r)$ may be seen as follows: The extreme value of $h_n(r)$ is defined by

$$|h_n(r)|\leqslant\lambda. \tag{20}$$

Since $\gamma_{k+\nu}<\gamma_k$, it is easily seen from Eq. (19) that

$$|\theta_{k+\nu}(n)|\leqslant\lambda^{\nu}|\theta_k(n)| \tag{21}$$

or that

$$\sum_{k=0}^{\infty}\theta_k(n)<\theta_0(n)\sum_{k=0}^{\infty}\lambda^k=\theta_0(n)/(1-\lambda)\quad\text{if}\quad\lambda<1, \tag{22}$$

which is to say that the sum (18) converges for $\lambda<1$. Now, since $f(r)>0$, except at $r=R$ where it vanishes, $h_n(r)<1$ as long as $\Delta_n(r)>0$; that is, as long as $V_n(r)<\phi(r)$. At $r=R$, application of L'Hospital's rule to the right-hand member of Eq. (17) shows that $h_n(R)=0$, in view of Eq. (7) and the fact that $V_n'(r)<0$. Since the *magnitude* of $h_n(r)$ is unaffected by changing the *sign* of $\Delta_n(r)$, it is clear that $|h_n(r)|<1$ as long as $V_n(r)<2\phi(r)$. This latter condition for the convergence of the sum (18) is sufficient, but not necessary. Since it is an easy matter to construct examples of $\phi(r)$ for which the sum does *not* converge, some caution is again warranted in applying these ideas to potentials more exotic than those discussed below. From the inequalities (21) and (22), the error of retaining the terms $k=0$, 1, $\cdots$, $K-1$ in the sum (18) is easily seen to be

$$\epsilon_K=\sum_{k=K}^{\infty}\theta_k(n)<\theta_K(n)/(1-\lambda)<\theta_0(n)\lambda^K/(1-\lambda) \tag{23}$$

as long as $\lambda<1$.

In the discussion thus far, it has been assumed that the parameters of the matching potential are evaluated according to (7) and are functions of both E_r and s. For many applications, a more convenient matching procedure replaces R in Eq. (7) by the distance of closest approach *in a head-on collision*: That is, the matching is carried out only for $s=0$, and α_n and β_n are retained for $s\neq 0$. This produces parameters depending only on E_r. The truncated Coulomb approximation discussed by Leibfried and Oen[11] is of this type, although they mention the possibility of the more general matching procedure also. The most familiar form of the hard core approximation[6] is also of this type. When "head-on" matching is used, the limits of the integrals in the expressions for $\theta_{\mathrm{app}}(n)$ and $\tau_{\mathrm{app}}(n)$ are no longer independent of n. Thus, although the order of the $V_n(r)$ is still correctly given by (14), one can no longer deduce (15) from it. The presence of a

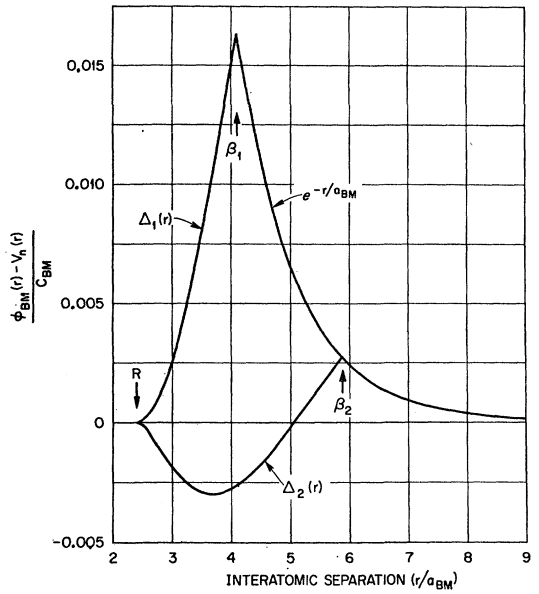

FIG. 3. The difference functions $\Delta_1(r)$ and $\Delta_2(r)$ for a Born-Mayer potential. $E_r=0.30\ C_{BM}$. $s=2\ a_{BM}$.

cutoff in the potential now affects the scattering: For $s \gtrsim \beta_n$, both $\theta_{app}(n)$ and $\tau_{app}(n)$ vanish. This cutoff complicates the discussion of just where the exact solutions stand in the sequence of approximations, but has the advantage for many purposes of producing a finite *total* cross section for scattering from these potentials. The perturbation expansion of these approximations has not been attempted, but numerical examples of their use will be given. If R in Eq. (7) is replaced by an *arbitrary* value of r, chosen as "typical," parameters can be derived which are independent of both E_r and s. This procedure produces the approximation used in early discussions of atomic slowing down problems in solids.[1,9]

III. NUMERICAL EXAMPLES

The approximations $\theta_{app}(n)$ and $\tau_{app}(n)$ can be evaluated in terms of elementary functions only for $n=1$, ± 2, and $-\infty$ (HC).[3] The necessary formulas, obtained by integrating Eqs. (1) and (2) with $\phi(r)$ replaced by $V_n(r)$, are collected in Appendix B. Instead of θ, most of the numerical tests employ the fractional transferred energy

$$T/T_{max}=\sin^2\theta/2\,, \tag{24}$$

where $T_{max}=4E_r/(1+A)$. The examples given are chosen to illustrate the surprising accuracy of the truncated Coulomb and truncated r^{-2} approximations, as well as to demonstrate some of the points discussed in the foregoing paragraphs. To emphasize the nature of the matching procedure, we will designate by $V_n{}^s(r)$ the approximations based on matching at $R(E_r,s)$ and by $V_n{}^0(r)$ the "head-on" approximations based on matching at $R(E_r,0)$. When no superscript is used, the remarks apply to both approximations equally.

For atomic interactions in solids, it is sometimes appropriate to use the exponential (Born-Mayer, Huntington) potential

$$\phi_{BM}(r)=C_{BM}\exp(-r/a_{BM})\,. \tag{25}$$

The approximation $V_n(r)$ is *plausible* for $R/a_{BM}>n$ and lies below $\phi_{BM}(r)$ for $R/a_{BM}>n+1$. Thus, only $V_{HC}(r)$ and $V_{-2}(r)$ are *always* plausible. Figure 3 shows plots of $\Delta_1(r)$ and $\Delta_2(r)$ for $\phi_{BM}(r)$, at $E_r=0.3\ C_{BM}$ (corresponding to an L kinetic energy of 13.5 keV for Cu-Cu interactions, if the parameters of potential II of Gibson *et al.*,[12] are used). The example is chosen to illustrate both a crossing ($\Delta_2<0$ sometimes) and a noncrossing ($\Delta_1>0$ always) approximate potential. Figure 4 shows the relative differences between the approximate and the exact[4] values of T/T_{max} for several approximate potentials. For small impact parameters, where $1<R/a_{BM}<2$, both $V_1{}^s$ and $V_1{}^0$ underestimate T/T_{max}. The implausibility region of $V_2{}^s$ is shown; the approximation $V_2{}^0$ is never plausible at this energy. The perturbation treatment is illustrated in Table I by computing the first two terms in the sum (18) for the $V_2{}^s$ approximation to $\phi_{BM}(r)$, at $E_r=0.05\ C_{BM}$ (corresponding to an L kinetic energy of about 2.2 keV for Cu-Cu interactions), and comparing these with the exact values of θ. The required term $\theta_1(2)$ is developed in Appendix C. It is evident that the first approximation is already very good and that most of the remaining discrepancy is removed by the next term in the series.

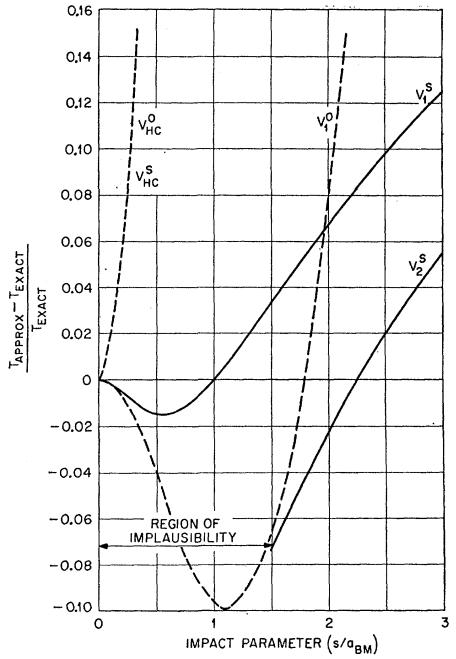

FIG. 4. Relative errors of some approximations to the transferred energy for the Born-Mayer potential. $E_r=0.30\ C_{BM}$.

[12] J. B. Gibson, A. N. Goland, M. Milgram, and G. H. Vineyard, Phys. Rev. **120**, 1229 (1960).

TABLE I. First- and second-order r^{-2} approximations to scattering from the Born-Mayer potential at $E_r=0.05\ C_{BM}$.

Impact parameter, s/a_{BM}	c.m. scattering angle, radians: Approximate $\pi-\theta_0(2)$	Approximate $\pi-\theta_0(2)-\theta_1(2)$	Exact θ
2	1.5255	1.5087	1.5048
3	0.9619	0.9387	0.9355
4	0.5579	0.5363	0.5337
5	0.2923	0.2758	0.2752
6	0.1382	0.1286	0.1284
7	0.0602	0.0559	0.0554
8	0.0249	0.0228	0.0227

Screened Coulomb potentials are of particular interest in atomic slowing down problems, since they have the correct limiting form (r^{-1}) for small interatomic separations. As long as the screening function $g_1(r)$ is always decreasing, the truncated Coulomb approximation, $V_1(r)$, is *plausible*; if $g_1''(r)>0$, $V_1(r)<\phi(r)$. The exponentially screened Coulomb (Bohr, Yukawa) potential,

$$\phi_B(r)=C_B(a_B/r)\exp(-r/a_B)\,, \tag{26}$$

which has been very widely used in radiation damage problems,[1,2,5–11] has both of these properties. The approximation $V_n(r)$ is plausible for $R/a_B>n-1$ and $V_n(r)<\phi_B(r)$ for $R/a_B>[n-1+(n-1)^{1/2}]$. Another screened Coulomb potential of interest is the Thomas-Fermi potential

$$\phi_{TF}(r)=C_{TF}(a_{TF}/r)\psi(r/a_{TF})\,, \tag{27}$$

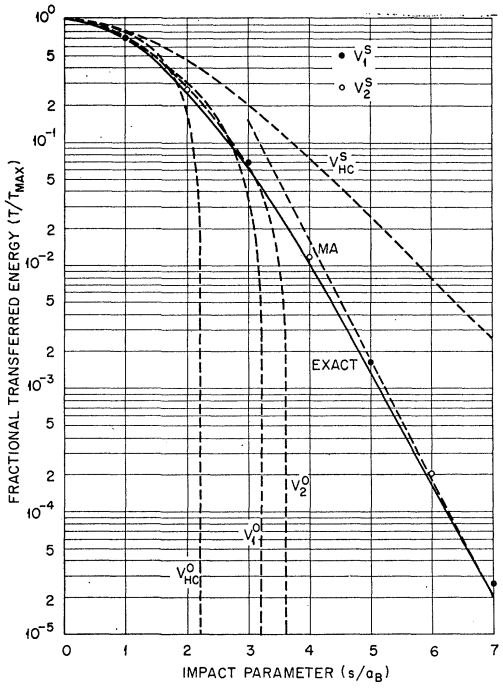

FIG. 5. Comparison of exact and approximate values of the fractional transferred energy for the Bohr potential. $E_r=0.05\ C_B$.

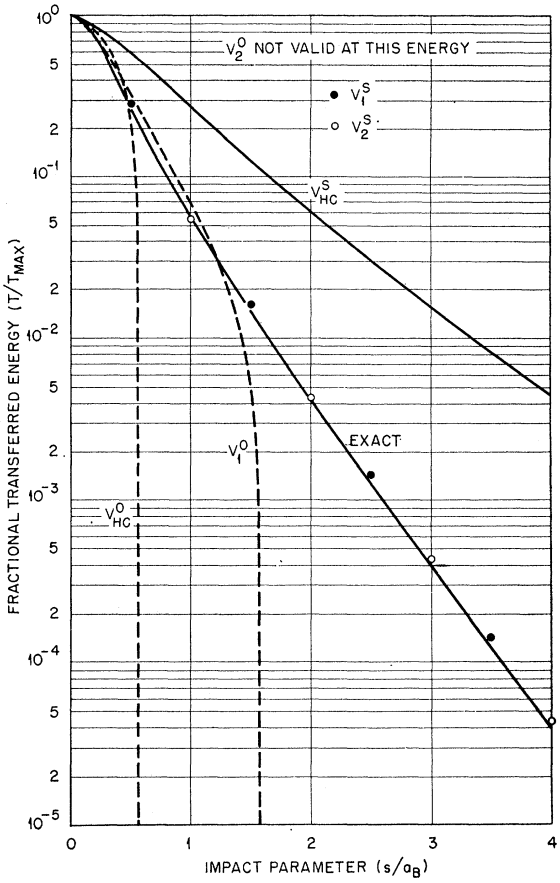

FIG. 6. Comparison of exact and approximate values of the fractional transferred energy for the Bohr potential. $E_r=1.0\ C_B$.

where $\psi(x)$ is the Thomas-Fermi screening function.[13] Since $\psi'(x)<0$, and $\psi''(x)>0$, $V_1(r)$ is always plausible and $<\phi_{TF}(r)$. Using Sommerfeld's approximation for $\psi(x)$ with March's parameters,[14] $V_2(r)$ is plausible for $R/a_{TF}>2.212$ and $<\phi_{TF}(r)$ for $R/a_{TF}>3.506$.

Several approximations to T/T_{max} are shown for the Bohr potential in Figs. 5 and 6. The energies correspond to L kinetic energies of about 10 and 200 keV, respectively, for Cu-Cu interactions, if Bohr's definition of a_B is used. Figures 7 and 8 show similar comparisons of the time integral τ. The excellence of the approximations V_1^s and V_2^s is apparent, particularly with respect to T/T_{max}. The two approximations differ from each other so little that the choice between them would be made on other grounds, such as the relative convenience of Eqs. (B.7) and (B.10) or the existence of an implausibility region in V_2^s. The superiority of the truncated Coulomb approximation V_1^0 to the usual hard-core approximation V_{HC}^0 is evident, as is the superiority of

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[14] A. Sommerfeld, Z. Physik **78**, 283 (1932); N. H. March, Proc. Cambridge Phil. Soc. **46**, 356 (1950).

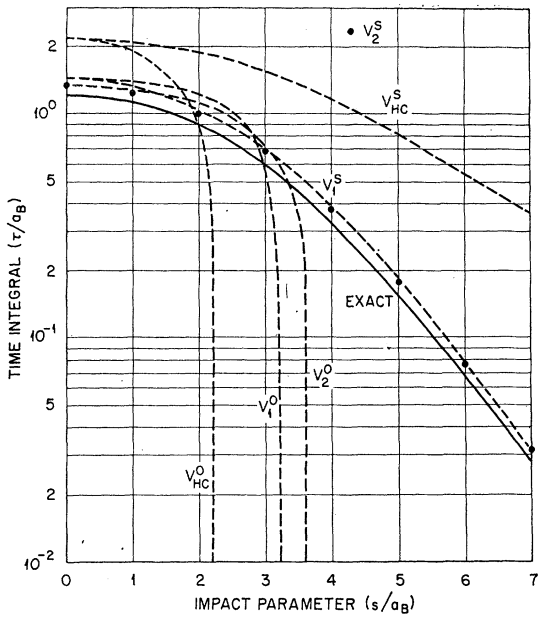

FIG. 7. Comparison of exact and approximate values of the "time integral" for the Bohr potential. $E_r=0.05\ C_B$.

V_2^0 to either of them. For large impact parameter, the MA is more accurate than any of the V_n approximations. Generally similar results (not presented here) have been obtained on comparison of the approximation V_1^s to the exact T/T_m for the Thomas-Fermi potential also. For all three of the potentials, Eqs. (25), (26), and (27), the *relative* error of the approximations to $T/T_{\max}$ increases with increasing impact parameter and with increasing energy (ignoring complications at high energy and small impact parameter caused by crossing of the approximate and exact curves). An upper limit to the relative error can be estimated from Eq. (23) with $K=1$. The real error actually will be smaller as one can learn from comparisons of the exact and approximate values of θ, T/T_m, and τ. The *absolute* error increases for small s, passes through a maximum and then decreases for large s. A similar behavior occurs for the absolute error as a function of E_r. The approximations to τ behave in a generally analogous manner. The accuracy of the approximate values of τ is less than that of the approximations to $T/T_{\max}$. This result was to be expected since the factor r^{-2} in the integral of Eq. (1) emphasizes the region in which the matching of $\phi(r)$ and $V_n(r)$ was done, whereas the absence of this factor in Eq. (2) causes the region of large r to assume greater importance.

IV. DISCUSSION

As has been shown earlier,[11] the approximation procedure based on matching $\phi(r)$ and $V_n(r)$ at $R(E_r,s)$ can be applied to the differential scattering cross section $K(T)$, as well as to θ, $T/T_{\max}$, and τ. Unfortunately, however, $K(T)$ can be expressed explicitly only as a function of R and not of T, as would be desired in applications, since, in general, analytical inversion of the relation $T=T(R)$ is not possible. In practical cases where $K(T)$ is of interest, as for instance in calculations of the stopping power, the general s-dependent matching is not necessarily an improvement over the s-independent matching at $R(E_r,0)$, because the crossing of θ and θ_{app} due to the cutoff nature of $V_n^0(r)$ can lead to a fortuitous improvement in $K(T)$.

The somewhat surprising result that for larger impact parameters the present approximations to $T/T_{\max}$ (or to θ) become less accurate than the MA is easily explained. If β_n-R were to vanish for large R, the perturbation $\Delta_n(r)$ would become identical to $\phi(r)$. In this circumstance, the expansion (18) in terms of $\Delta_n(r)$ would become the same as the MA expansion[2] in terms of $\phi(r)$. The term $\theta_1(n)$ would then correspond to the (first) MA. In fact, for the potentials (25) and (26), β_n-R remains finite (and equal, respectively, to a_{BM} or a_B) for large R. Thus, the result of Fig. 5 that the MA is more accurate than either V_1^s or V_2^s merely means that the correction term $\theta_1(n)$ becomes more significant for large s, as is also evident from Table I. Since the matching potential method is superior for small s, as is the MA for large s, the two approximations supplement each other. However, for the restricted range of impact parameters occurring in crystals, the matching potential method is mostly superior to the MA.

Extension of the matching potential method to the treatment of the complete trajectories of two interacting particles (instead of only to their asymptotes) is straightforward. The complete trajectories may be given in c.m. polar coordinates in terms of Eqs. (1) and (2) and of additional similar equations in which the infinite

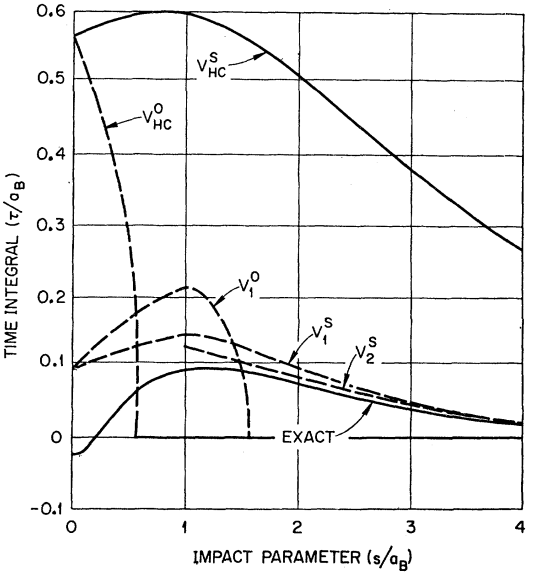

FIG. 8. Comparison of exact and approximate values of the "time integral" for the Bohr potential. $E_r=1.0\ C_B$.

upper limits of the two integrals are replaced by the values of r, the c.m. radial coordinate. A further possible extension of the matching potential method would involve the use of sums of power potentials, such as

$$V(r)=\alpha/r^2+\beta/r+\gamma,$$

for which the scattering integrals remain elementary. Attempts to use this form, with the contants evaluated by matching $\phi(R)$, $\phi'(R)$, and $\phi''(R)$, have not been fruitful, however.

Besides advantages in handling scattering problems analytically, the matching potential procedure discussed here also would provide a simplification in the numerical treatment of complicated slowing down problems in solids where a great many subsequent collisions have to be considered.[15] The time required by an electronic computer for this kind of problem can be considerably reduced without significant loss of accuracy.

The approximations which have been discussed make it feasible to attack some problems closely related to radiation damage in crystalline structures: Small angle focusing collisions[16] can be pursued to larger angles, assisted focusing collisions[17] can be handled without the limitations of the MA, and channeling events[18] can be investigated for larger amplitudes. These are the objectives of future work.

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APPENDIX A

The Zeros of $\Delta_n(r)$

The slope and curvature of the difference function $\Delta_n(r)$ may be written from Eqs. (6) and (12) as

$$\Delta_n'(r)=\phi'(r)-\phi'(R)(R/r)^{n+1} \qquad R<r<\beta_n \quad \text{(A1)}$$

$$\Delta_n''(r)=\phi''(r)+(n+1)[\phi'(R)/R](R/r)^{n+2} \qquad R<r<\beta_n. \quad \text{(A2)}$$

It is evident that $\Delta_n''(R)>0$ as long as

$$R\phi''(R)>-(n+1)\phi'(R) \quad \text{or}$$
$$Rg_n''(R)>(n-1)g_n'(R). \quad \text{(A3)}$$

Thus, since $\Delta_n(\beta_n)>0$, $\Delta_n(r)$ has an even number of zeros in $R<r<\beta_n$ (in addition to the one at $r=R$) as long as (A3) holds. If (A3) does not hold, the number of zeros is odd. Although the occurrence of these zeros can be examined in $\Delta_n(r)$ itself, it is more convenient to use the fact that, as long as they are all real, they are separated by (or coincide with) the zeros of $\Delta_n'(r)$. These latter are given by the solutions of

$$r^{n+1}\phi'(r)=R^{n+1}\phi'(R) \quad \text{(A4)}$$

which has an obvious solution $r=R$. There can be additional solutions if the left-hand member of (A4) has extrema, that is, if there exist solutions of

$$r\phi''(r)=-(n+1)\phi'(r) \quad \text{(A5)}$$

for $R<r<\beta_n$. Thus, the study of Eq. (A5) may substitute for that of $\Delta_n(r)$ itself. Note that (A3) becomes an equality when $r=R$ is a solution of (A5). This condition, under which $\Delta_n''(R)$ vanishes, separates two regions, in one of which $\Delta_n''(R)>0$ and $V_n(r)<\phi(r)$ near $r=R$, while for the other, $\Delta_n''(R)<0$ and $V_n(r)>\phi(r)$ near $r=R$. Hence, the occurrence of $r=R$ as a solution to Eq. (A5) represents the critical condition for $V_n(r)$ to cross $\phi(r)$. For potentials $\phi(r)$ for which $g_n(r)=r^n\phi(r)$ can be found so that $g_n'(r)<0$ and $g_n''(r)>0$ in the interval $R<r<\beta_n$, the approximation $V_n(r)$ will be both plausible and always $\leq\phi(r)$. This situation is true of the potentials considered in this communication.

APPENDIX B

Scattering Integrals for Approximate Potentials

The scattering integrals (1) or (24) and (2) are collected here for the readily integrable potentials $V_n(r)$ with $n=1$, ±2, and $-\infty$ (HC). In each case, the quantity given vanishes outside the range $0<s<\beta_n$. (Of course, when β_n is a function of s, $s>\beta_n$ can never occur.) The following abbreviations are used:

$$\sigma=s/\beta_n \quad \text{and} \quad \gamma=\alpha_n/|n|E_r. \quad \text{(B1)}$$

Hard-core approximation ($n=-\infty$):

$$T/T_{\max}=1-s^2/R^2 \quad \text{(B2)}$$

$$\tau=(R^2-s^2)^{1/2}. \quad \text{(B3)}$$

Quadratic approximation ($n=-2$):

$$\theta=2\cos^{-1}\sigma+\cos^{-1}[(\gamma-1+2\sigma^2)/\rho] \quad \text{(B4)}$$

$$\tau/\beta_{-2}=(1-\sigma^2)^{1/2}-(\gamma^{-1/2}/2)\times\ln\{[1+\gamma+2\gamma^{1/2}(1-\sigma^2)^{1/2}]/\rho\}, \quad \text{(B5)}$$

where

$$\rho^2=(\gamma-1)^2+4\gamma\sigma^2. \quad \text{(B6)}$$

Truncated Coulomb approximation ($n=1$):

$$T/T_{\max}=(1-\sigma^2)/\rho^2 \quad \text{(B7)}$$

$$\tau(1+\gamma)/\gamma\beta_1=(1-\sigma^2)^{1/2}-[(1+\gamma)^{-1/2}/2]\times\ln(\{2+\gamma+2[(1+\gamma)(1-\sigma^2)]^{1/2}\}/\gamma\rho) \quad \text{(B8)}$$

where

$$\rho^2=1+4\sigma^2(1+\gamma)/\gamma^2. \quad \text{(B9)}$$

[15] M. T. Robinson and O. S. Oen, Phys. Rev. **132**, 2385 (1963).
[16] C. Lehmann and G. Leibfried, Z. Physik **162**, 203 (1961).
[17] P. H. Dederichs and G. Leibfried, Z. Physik **170**, 320 (1962).
[18] C. Lehmann and G. Leibfried, J. Appl. Phys. **34**, 2821 (1963).

Truncated r^{-2} approximation ($n=2$):

$$\theta/2=\cos^{-1}\sigma-[\sigma/(\gamma+\sigma^2)^{1/2}]\times\cos^{-1}[(\gamma+\sigma^2)/(1+\gamma)]^{1/2} \quad \text{(B10)}$$
$$\tau/\beta_2=[\gamma/(1+\gamma)](1-\sigma^2)^{1/2}.$$

APPENDIX C

Evaluation of $\theta_1(2)$ for the Born-Mayer Potential

For the special case of the potential (25) matched by $V_2{}^s(r)$, the definition (19) gives

$$\begin{aligned}\theta_1(2)&=s\int_R^\infty dr[\phi_{\rm BM}(r)-V_2(r)]/E_r r^2[f_2(r)]^3\\&=[s\phi_{\rm BM}(\beta_2)/E_r][(\beta_2{}^2-s^2)^{-1/2}\\&\quad-(1+\alpha_2/2E_r)^{-3/2}(\beta_2{}^2-R^2)^{-1/2}]\\&\quad-(1+\alpha_2/2E_r)^{-3/2}(sC_{\rm BM}/a_{\rm BM}E_r)\\&\quad\times\bar{E}[R/a_{\rm BM},(\beta_2{}^2+R^2)^{1/2}/a_{\rm BM}]\\&\quad+(1+\alpha_2/2E_r)^{-3/2}(\alpha_2 s\beta_2/2E_r R^2)\\&\quad\times\{[(\beta_2/R)^2-1]^{1/2}+(\beta_2/R)\cos^{-1}(R/\beta_2)\}\\&\quad-(sC_{\rm BM}/a_{\rm BM}E_r)[K_0(s/a_{\rm BM})\\&\qquad-\bar{E}(s/a_{\rm BM},(\beta_2{}^2+s^2)^{1/2}/a_{\rm BM}].\end{aligned} \quad \text{(C1)}$$

In this expression, $K_0(\alpha)$ is the well-known Hankel function and $\bar{E}(\alpha,x)$ is one of the generalized exponential integral functions:

$$\bar{E}(\alpha,x)=\int_0^x (dy/u)e^{-u}=\sinh^{-1}(x/\alpha)-E(\alpha,x), \quad \text{(C2)}$$

where $u=(\alpha^2+y^2)^{1/2}$. Note that $K_0(\alpha)=\bar{E}(\alpha,\infty)$. In Eq. (C2), the function $E(\alpha,x)$ is a generalized exponential integral function which has been tabulated.[19] For large impact parameters, the necessity of double interpolation in the tables of $E(\alpha,x)$ makes their use difficult and it is more convenient to use an expansion of the integral (C2). With the substitution $u=\eta^2+\alpha$, Eq. (C2) yields

$$\bar{E}(\alpha,x)=(2/\alpha)^{1/2}e^{-\alpha}\int_0^{\lambda^{1/2}} d\eta e^{-\eta^2}(1+\eta^2/2\alpha)^{-1/2}, \quad \text{(C3)}$$

where $\lambda=(x^2+\alpha^2)^{1/2}-\alpha$. As long as $\eta^2/2\alpha<1$, the binomial in (C3) may be expanded; that is, as long as $x^2<8\alpha^2$. Inserting the appropriate arguments from Eq. (C1), the requirement becomes $\beta_2{}^2<7R^2$ or $\beta_2{}^2<7s^2$, respectively, in the two integrals. Both conditions are met for sufficiently large values of s. After expanding (C3) and integrating, there results

$$\begin{aligned}\bar{E}(\alpha,x)&=(\pi/2\alpha)^{1/2}e^{-\alpha}\,\mathrm{erf}(\lambda^{1/2})\\&\quad\times\{1-(1/8\alpha)[1-2(\lambda/\pi)^{1/2}e^{-\lambda}/\mathrm{erf}(\lambda^{1/2})]\\&\quad+(9/128\alpha^2)[1-2(\lambda/\pi)^{1/2}e^{-\lambda}\\&\qquad\times(1+2\lambda/3)/\mathrm{erf}(\lambda^{1/2})]-+\ldots\},\end{aligned} \quad \text{(C4)}$$

where

$$\mathrm{erf}x=2\pi^{-1/2}\int_0^x du\exp(-u^2)$$

is the error function. The series (C4) has the advantage of involving only functions of single variables. Since it is alternating in sign, the error of retaining only a finite number of terms is less than the first term omitted.

[19] Harvard University Computation Laboratory, *Tables of the Generalized Exponential-Integral Functions* (Harvard University Press, Cambridge, Massachusetts, 1949).