Focusing Collisions in a Linear Chain of Atoms*

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Focusing of the Silsbee type is studied in a row of identical atoms with the uniform spacing S, which interact during collisions through a repulsive potential $V(r)$. Two energy-dependent parameters are introduced: the distance of closest approach in a head-on collision c, and $\gamma=-(d\ln V/d\ln r)_{r=c}$. In terms of these, the focusing parameter $\Lambda=\theta_2/\theta_1$ is approximately $(SI_0/c)-1$, where I_0 is an integral involving $V(r)$ which depends mainly on γ. For simple exponential potentials and large γ, $I_0=1+(\ln 4)/\gamma-1.368/\gamma^2+3.41/\gamma^3\cdots$. Appreciably less focusing is predicted than follows from earlier approximations which correspond to putting $I_0=1$. For ⟨110⟩ chains in copper, focusing is found at energies below 23 ev. This compares well with the 30 ev obtained by Gibson *et al.*, for their three-dimensional model of copper.

INTRODUCTION

In early calculations on irradiation effects in solids, correlations which might result from the regular lattice structure were almost entirely ignored. The likelihood of an important focusing effect, leading to the propagation of energy pulses along close-packed rows of atoms, was apparently first demonstrated by Silsbee.[1] His expectations have been confirmed by later research, particularly by the extensive calculations of Gibson *et al.*[2] on the dynamics of radiation damage in a model representing copper.

Gibson *et al.* compare some of the focusing results for their three-dimensional model with an approximate analysis of a linear chain. This latter analysis follows a common practice, treating the scattering as though the atoms were spheres with diameters equal to the distance of closest approach in a head-on collision. This approximation overestimates the equivalent sizes of the atoms and predicts too strong focusing. In the present paper, a more accurate, but still rather simple analysis, is developed by looking more carefully at classical scattering relations, particularly for nearly head-on collisions.

FORMULATION OF THE PROBLEM

Consider a long row of identical, uniformly spaced atoms, S being the distance between neighbors. Let an atom be set in motion with a kinetic energy E and at a small angle θ_1 with the line of centers. The target atom will be driven away at some angle θ_2 with the line of centers. When E is sufficiently large (perhaps a few electron volts or more) the event may be treated approximately as an isolated collision between two atoms which interact through a repulsive potential energy $V(r)$.

The classical relation between the scattering angle in center-of-mass coordinates θ and the impact parameter $p=S\sin\theta_1$ can be written in the form $\theta=\pi-(2pI/c)$, where c is the distance of closest approach in a head-on collision, and

$$I=\int_{x_0}^{\infty}[1-(p/cx)^2-v(x)]^{-\frac{1}{2}}x^{-2}dx. \tag{1}$$

Here $x=r/c$, $v(x)=V(r)/V(c)$, and $r_0=cx_0$ is the distance of closest approach for the impact parameter p. On the other hand, from conservation of energy and momentum: $\theta=\pi-2(\theta_1+\theta_2)$. These two expressions for θ lead to the focusing parameter

$$\Lambda=\theta_2/\theta_1=(IS\sin\theta_1/c\theta_1)-1. \tag{2}$$

When θ_1 is small, this reduces to

$$\Lambda=(SI_0/c)-1, \tag{3}$$

where

$$I_0=\int_1^{\infty}[1-v(x)]^{-\frac{1}{2}}x^{-2}dx. \tag{4}$$

When Λ is less than unity each atom moves off at a smaller angle with the line of centers than did its predecessor.

It should be noted that I_0 and the differential cross section for $\theta=\pi$ are closely related. In general

$$\sigma(\theta)=-pdp/\sin\theta d\theta=pc\{[2d(pI)/dp]\sin(2pI/c)\}^{-1}. \tag{5}$$

When p approaches zero, this reduces to $\sigma(\pi)=(c/2I_0)^2$.

EVALUATION OF I_0

It is desirable to consider together all potentials of the form

$$V=Br^{-n}\exp(-r/a), \tag{6}$$

where B and a are positive and n is positive or zero. In addition to c, a second energy-dependent parameter $\gamma=-(d\ln V/d\ln r)_{r=c}$ may be introduced.[3] One then

* Supported by the Aeronautical Research Laboratories, Wright Air Development Division. A brief report of these results was made earlier [E. M. Baroody, Bull. Am. Phys. Soc. **6**, 293 (1961)].

[1] R. H. Silsbee, J. Appl. Phys. **28**, 1246 (1957).

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

[3] The idea of introducing a parameter γ defined in this way was suggested by the remarks of Bohr concerning the value of comparing the scattering by exponentially screened Coulomb potentials with that by inverse power law potentials. [N. Bohr, Kgl. Danske Videnskab. Selskab., Math.-fys. Medd. **18**, No. 8 (1948).]

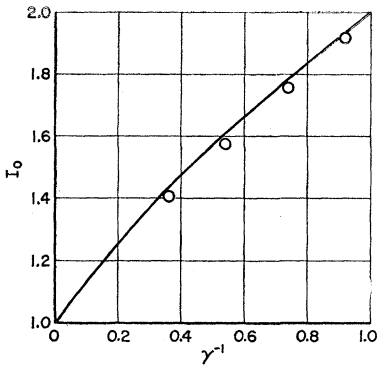

FIG. 1. Behavior of the integral I_0 for $n \geqslant 1$. The line is for power laws ($n=\gamma$) and was computed from Eq. (12). The points are for exponentially screened Coulomb potentials ($n=1$), and are based on results of Everhart, Stone, and Carbone. (For $n>1$, results would be confined to the range $\gamma^{-1}<n^{-1}$, and would lie between those for power laws and for $n=1$.)

finds from Eq. (6), $\gamma=n+(c/a)$ and

$$v(x)=x^{-n}\exp[-(\gamma-n)(x-1)]. \quad (7)$$

When γ is substantially larger than unity (the range of greatest interest here), the form of $v(x)$ is largely determined by γ alone, the value of n becoming important only where $v(x)$ is small. In this case it is convenient to introduce $z=-\ln v$, and use Eq. (7) to obtain

$$x=1+z/\gamma+nz^2/2\gamma^3+n(3n-2\gamma)z^3/6\gamma^5+,\cdots. \quad (8)$$

Substitution into Eq. (4) leads to

$$I_0=1+D_0/\gamma-(2\gamma-n)D_1/\gamma^3 + (6\gamma^2-8n\gamma+3n^2)D_2/2\gamma^5+\cdots, \quad (9)$$

where

$$D_k=\frac{1}{2(k+1)}\int_0^\infty z^{k+1}\exp(-z)[1-\exp(-z)]^{-\frac{3}{2}}dz. \quad (10)$$

An elementary integration gives $D_0=\ln 4$. On the other hand, expansion of the denominator of the integrand leads to a formula which converges rapidly for large k:

$$D_k=(k!/2)[1+(3/8)(2^{-k})+(5/24)(3^{-k})+\cdots]. \quad (11)$$

A convenient way to evaluate D_1 and D_2 is to consider the inverse power law potentials ($a=\infty$, $\gamma=n$). For this case, a well-known integral involving gamma functions is obtained:

$$I_0=(\pi)^{\frac{1}{2}}\gamma^{-1}\Gamma(\gamma^{-1})/\Gamma(\gamma^{-1}+0.5). \quad (12)$$

Use of expansions for the gamma functions and comparison with Eq. (9) leads to $D_1=0.684$ and $D_2=1.136$.

A careful discussion of the convergence properties of Eq. (9) will not be given here. A casual inspection indicates, however, that for the inverse power law potentials the expansion is convergent when γ is greater than unity, while for the other cases it is an asymptotic expansion which gives results correct to less than three percent for $\gamma \gtrsim 5$.

It is obvious from Eq. (9) that for large γ, I_0 is approximately the same for all the potentials included in Eq. (6). It is also true that for $n \gtrsim 1$, I_0 is approximately independent of n for all possible γ. This is illustrated in Fig. 1, where I_0 is plotted against γ^{-1}. The line is computed for power laws from Eq. (12), while the circles apply to exponentially screened Coulomb potentials ($n=1$), and follow from the results of Everhart *et al.*[4]

It has been seen here that expansion in inverse powers of γ provides useful approximations for I_0 and $\sigma(\pi)$. By expanding the general integral of Eq. (1), one can also derive approximations for $\sigma(\theta)$ which are useful over a wide range of angles. A brief discussion of this topic is being published elsewhere.[4a]

APPLICATION TO ⟨110⟩ CHAINS IN COPPER[5]

For most of their calculations on copper, Gibson *et al.*, used an exponential potential with $B=22\,600$ ev and $a=d/13$, where d is the distance between nearest neighbors. These constants imply $c=\gamma d/13$ and γ

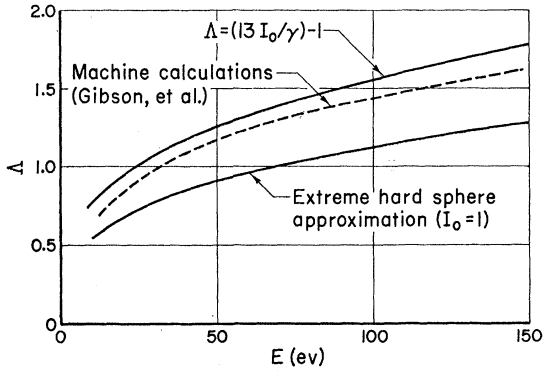

FIG. 2. Focusing parameter $\Lambda=\theta_2/\theta_1$ as a function of energy for ⟨110⟩ chains in copper.

[4] E. Everhart, G. Stone, and R. J. Carbone, Phys. Rev. **99**, 1287 (1955). These authors report extensive numerical calculations on scattering by exponentially screened Coulomb potentials. Their tables include differential cross sections for a number of cases of light and moderate screening ($\gamma \lesssim 2.75$).

[4a] E. M. Baroody, Phys. Fluids **4**, 1182 (1961).

[5] After this paper was completed the author's attention was called to a treatment of focusing in ⟨110⟩ chains published recently by C. Lehmann and G. Leibfried [Z. Physik, **162**, 203 (1961)]. They corrected the usual hard-sphere expression for the focusing parameter Λ in two steps. The first replaced the hard-sphere radius by an effective radius which is the same as c/I_0 of the present paper. They next showed that the atomic separation S should be replaced by a slightly smaller distance. Their final formula gives a curve of Λ against E which runs just a little below the machine calculations, thus showing that the influence of neighboring chains can be neglected. For an exponential potential they evaluated I_0 in terms of c/a, obtaining the same asymptotic expansion found here, although their handling of the coefficients was a bit different. They did not consider other analytic forms of the potential, or comment on the relation between I_0 and differential cross sections.

$=10.72-\ln E$, where E is in electron volts. For the $\langle 110\rangle$ chains $S=d$ and Eq. (3) becomes $\Lambda=(13I_0/\gamma)-1$. The upper solid curve in Fig. 2 follows from this relation with I_0 computed from Eq. (9) with $n=0$. The dashed curve shows the trend of Λ with energy as revealed by the calculations of Gibson *et al.* (see their Fig. 27). The agreement is satisfactory, the slightly greater focusing found in the three-dimensional model probably resulting from the effect of neighboring chains of atoms. The lower curve in Fig. 2 corresponds to $I_0=1$, that is, to the commonly used equivalent hard-sphere approximation.

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Anharmonic Contribution to the Energy of a Dilute Electron Gas—Interpolation for the Correlation Energy

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The first anharmonic contribution to the ground-state energy of a body-centered cubic lattice of electrons, oscillating in a uniform background positive charge, has been calculated. The result is $-0.73r_s^{-2}$ rydbergs, with r_s the radius, in Bohr units, of the sphere equivalent in volume to that occupied per electron. Combining this term with previous results gives for the ground-state energy of a dilute electron gas the expression $E=E_{\rm exp}-1.792r_s^{-1}+2.65r_s^{-\frac{3}{2}}-0.73r_s^{-2}+O(r_s^{-\frac{5}{2}})$, where $E_{\rm exp}$ comes from the overlapping of electronic wave functions and falls off exponentially with $r_s^{\frac{1}{2}}$; while the r_s^{-1} and $r_s^{-\frac{3}{2}}$ terms are, respectively, the Coulomb energy of a bcc lattice and the zero-point energy of the electrons.

The "correlation" energy corresponding to the above expression, as well as the kinetic and potential parts, has been plotted and an interpolation has been made between the low-density curve and the high-density expression of Gell-Mann and Brueckner. The interpolated curves give strong evidence that the next term in the above low-density expansion for E is approximately $-0.8r_s^{-\frac{5}{2}}$. If the high-density expression is rapidly converging near $r_s=1$, it also is predicted that the r_s term in the high-density expansion will be approximately $-0.02r_s$.

WIGNER[1] originally pointed out that the ground-state energy of an electron gas (electrons moving in a uniform background of positive charge) approaches the energy for a body-centered cubic lattice of electrons as the density approaches zero. This energy, as calculated by Fuchs,[2] is $-1.792r_s^{-1}$ rydbergs per electron, where r_s is, in Bohr units, the radius of a sphere equal in volume to the volume per electron of the gas. The next approximation to the energy of the dilute gas is obtained from the zero-point motion of the electrons about their lattice points, which becomes a problem of evaluating the normal modes of the oscillations. Recently, two accurate calculations for the zero-point motion have been made independently,[3,4] the results agreeing within one percent. We shall take the average of these two results, $2.65r_s^{-\frac{3}{2}}$, which may be compared with the values $3r_s^{-\frac{3}{2}}$ and $2.7r_s^{-\frac{3}{2}}$ obtained by Wigner[1] from two different estimates.

A complete solution of the lattice dynamics which is encountered in the dilute electron gas problem is obtained by expanding the Coulomb potential in powers of displacements of the electrons about their respective lattice points. The energy then is an infinite series in powers of $r_s^{-\frac{1}{2}}$, the terms beyond the $r_s^{-\frac{3}{2}}$ term being the anharmonic corrections, which may be calculated from perturbation theory. The first anharmonic correction, the r_s^{-2} term, comes from the sum of a second-order energy perturbation due to cubic terms in the displacements, and the first-order perturbation due to the quartic terms in displacements.

From Appendix II of reference 4, the cubic and quartic terms lead, respectively, to the energy expressions (in rydbergs), per electron:

$$\epsilon_3=-\left(\frac{3}{\pi}\right)^{8/3}\frac{r_s^{-8}}{24}N^{-2}\sum_{\mathbf{f}\mathbf{f}'ss's''}|B(\mathbf{f},\mathbf{f}',s,s',s'')|^2 \times[\omega(\mathbf{f},s)\omega(\mathbf{f}',s')\omega(\mathbf{f}+\mathbf{f}',s'']^{-1} \times[\omega(\mathbf{f},s)+\omega(\mathbf{f}',s')+\omega(\mathbf{f}+\mathbf{f}',s'')]^{-1}, \quad (1)$$

and

$$\epsilon_4=\left(\frac{3}{\pi}\right)^{5/3}\frac{r_s^{-5}}{8}N^{-2}\sum_{\mathbf{n}\neq 0}\left[\sum_{\mathbf{f},s}\frac{D_{\mathbf{n}}(\mathbf{f},s)}{\omega(\mathbf{f},s)}\right]^2\frac{1}{n}, \quad (2)$$

where

$$B=\sum_{\mathbf{n}\neq 0}[\sin\mathbf{f}\cdot\mathbf{n}+\sin\mathbf{f}'\cdot\mathbf{n}-\sin(\mathbf{f}+\mathbf{f}')\cdot\mathbf{n}][\mathbf{v}(\mathbf{f},s)\cdot\nabla_n] \times[\mathbf{v}(\mathbf{f}',s')\cdot\nabla_n][\mathbf{v}(\mathbf{f}-\mathbf{f}',s'')\cdot\nabla_n]\frac{1}{n}, \quad (3)$$

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[1] E. P. Wigner, Phys. Rev. **46**, 1002 (1934); Trans. Faraday Soc. **34**, 678 (1938).

[2] K. Fuchs, Proc. Roy. Soc. (London) **A151**, 585 (1935).

[3] Rosemary Coldwell-Horsfall and A. A. Maradudin, J. Math. Phys. **1**, 395 (1960).

[4] W. J. Carr, Jr., Phys. Rev. **122**, 1437 (1961).