

The Elastic Scattering of Low Energy Electrons in Thomas-Fermi Theory

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A detailed study has been made of the elastic scattering of low-energy electrons in Thomas-Fermi Theory. The analytical expressions which have been obtained for the scattering length a and the total cross section σ are illustrated numerically.

The purpose of this paper is to give accurate analytical expressions for the scattering length a and the total cross-section σ for elastic scattering of low energy electrons by atoms.

In atomic units, the Schrödinger equation for the s-states for the approximate Thomas-Fermi potential¹ given by the author² has the following form

$$y_0(r) = r {}_2F_1 \left[\frac{1}{2} + \frac{1}{2} \left(1 + \frac{8Z}{A-B} \right)^{1/2}, \frac{1}{2} - \frac{1}{2} \left(1 + \frac{8Z}{A-B} \right)^{1/2}, 2; \frac{(A-B)r}{(1+A)r} \right] \quad (2)$$

where ${}_2F_1$ denotes the hypergeometric function. If we compare the solution given by Eq. (2) for $r \rightarrow \infty$ with the free solution ($Z=0$), we see that, for large values of r , $y_0(r)$ must have the asymptotic form

$$y_0(r) \xrightarrow{r \rightarrow \infty} C(r-a). \quad (3)$$

Using this formula we obtain the following expres-

$$y'' + \left[k^2 + \frac{2Z}{r(1+A)r^2(1+B)r} \right] y = 0 \quad (1)$$

sion for the scattering length a where $A=0.53652 Z^{1/3}$ and $B=0.044081 Z^{1/3}$. This equation has the advantage that one can solve it exactly for $k=0$. If we denote by y_0 the solution for $k=0$ which fulfills the boundary condition $y_0(0)=0$, we see that $y_0(r)$ is given by³

sion for the scattering length a

$$a = \lim_{r \rightarrow \infty} \frac{r^2 {}_2F_1'(r)}{{}_2F_1(r)} \quad (4)$$

where ${}_2F_1'$ denotes the first derivative of ${}_2F_1$. Using Eq. (1) for $k=0$ and the corresponding free equation $\bar{y}_0''=0$ one can obtain equivalent formula for the scattering length

$$a = - \frac{2Z}{\left[{}_2F_1 \left[\frac{1}{2} + \frac{1}{2} \left(1 + \frac{8Z}{A-B} \right)^{1/2}, \frac{1}{2} - \frac{1}{2} \left(1 + \frac{8Z}{A-B} \right)^{1/2}, 2; \frac{(A-B)r}{A} \right] \right]} \cdot \int_0^\infty \frac{y_0(r) dr}{(1+A)r^2(1+B)r} \quad (5)$$

where $y_0(r)$ is given by Eq. (2). Simple calculations show that Eqs. (4) and (5) give the same results for the scattering length a given by

$$a = - \frac{Z}{A^2} \frac{{}_2F_1 \left[\frac{3}{2} + \frac{1}{2} \left(1 + \frac{8Z}{A-B} \right)^{1/2}, \frac{3}{2} - \frac{1}{2} \left(1 + \frac{8Z}{A-B} \right)^{1/2}, 3; \frac{A-B}{A} \right]}{{}_2F_1 \left[\frac{1}{2} + \frac{1}{2} \left(1 + \frac{8Z}{A-B} \right)^{1/2}, \frac{1}{2} - \frac{1}{2} \left(1 + \frac{8Z}{A-B} \right)^{1/2}, 2; \frac{A-B}{A} \right]}. \quad (6)$$

The last equation gives us an analytical expression for the scattering length a as a function of atomic number Z . Using Eq. (1) for $y(r)$ the free equation for $\bar{y}(r)$ and the corresponding equation for $y_0(r)$ and $\bar{y}_0(r)$ we obtain after simple calculations the

following formula for the phase shift $\delta(k)$ given below.

$$\delta(k) = -ka. \quad (7)$$

The last formula is valid for very small k -values. The cross-section σ as known is given by the rela-

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¹ P. GOMBÁS, Encyclopedia of Physics, ed. S. FLÜGGE, Springer-Verlag, Berlin 1956, Vol. 36.

² T. TIETZ, Nuovo Cim. 28, 1509 [1963].

³ T. TIETZ, Z. Naturforsch. 21 a, 360 [1966].



tion

$$\sigma = \int_0^{4\pi} |f(\Theta, \Phi)|^2 d\Omega \quad (8)$$

where $f(\Theta, \Phi)$ is the amplitude of the scattered wave. For s-states the scattering amplitude $f(\Theta, \Phi)$ as known is

$$f(k, 0) = \frac{e^{2i\delta(k)} - 1}{2ki} = \frac{e^{i\delta(k)}}{k} \cdot \sin \delta(k). \quad (9)$$

Using formula (7), (8) and (9) we obtain for $k \rightarrow 0$

$$\sigma = 4\pi f^2(0, 0) = 4\pi a^2. \quad (10)$$

One sees from the last equation that the amplitude of the scattered wave for zero energy incident electrons is an equivalent definition of the scattering length a and according to Eqs. (7) and (9) given by $a = -f(0, 0)$.

For $k \neq 0$ but very small using Eq. (7) and (9) we obtain for the scattering amplitude $f(k, 0)$ the relation

$$f(k, 0) = -a e^{-ika} = -a(1 - ika). \quad (11)$$

We see from Eq. (7) for $\delta(k)$ and Eq. (11) for $f(k, 0)$ valid for very small k -values that $\delta(k)$ and $f(k, 0)$ fulfill the correct relations

$$\delta(-k) = -\delta(k), \quad f(k, 0) = f^*(-k, 0). \quad (12)$$

Substituting $f(k, 0)$ given by Eq. (11) into Eq. (8) for σ we obtain

$$\sigma = 4\pi a^2(1 - k^2 a^2) \quad (13)$$

valid for very small k -values.

In Table 1 we have collected the numerical values of a given by Eq. (6) from $Z=2$ to $Z=100$. The scattering length a has been evaluated by a computer.

Table 1 shows that the scattering length a is not monotonic function of the atomic number Z but rather a periodic function of Z . The scattering length a according to this table has very high values if $Z=12, 19, 31, 38, 47, 58, 59, 85, 86, 94, 95$, and 96. The sign and magnitude of the scattering length are very important if we wish to study the elastic scattering of low energy electrons by atoms and the shape of the cross-section σ . Since Eq. (13) for σ is valid for very small k -values so far such atomic numbers Z for which the scattering length a is very large we can expect for small k -values the typical Ramsauer-Townsend effect. Another physical explanation if a is positive or negative but very large can be found by MESSIAH⁴ in his book.

Since the scattering length is given analytically we can calculate the phase shifts δ using the theory of LEVY and KELLER⁵. In any case the phase shifts

Z	a	Z	a	Z	a	Z	a
2	$-0.125780 \cdot 10^2$	26	$-0.311994 \cdot 10^2$	51	$-0.117182 \cdot 10^3$	76	$-0.115907 \cdot 10$
3	$-0.144506 \cdot 10^2$	27	$-0.316475 \cdot 10^2$	52	$+0.798201 \cdot 10^2$	77	$-0.151320 \cdot 10$
4	$-0.159566 \cdot 10^2$	28	$-0.320869 \cdot 10^2$	53	$+0.309191 \cdot 10^2$	78	$-0.210382 \cdot 10$
5	$-0.102137 \cdot 10^2$	29	$-0.325177 \cdot 10^2$	54	$+0.194685 \cdot 10^2$	79	$-0.264030 \cdot 10$
6	$-0.183715 \cdot 10^2$	30	$-0.329407 \cdot 10^2$	55	$+0.142963 \cdot 10^2$	80	$-0.323500 \cdot 10$
7	$-0.193914 \cdot 10^2$	31	$-0.624738 \cdot 10^{18}$	56	$+0.113076 \cdot 10^2$	81	$-0.390471 \cdot 10$
8	$-0.203253 \cdot 10^2$	32	$+0.383114 \cdot 10$	57	$+0.933309 \cdot 10^2$	82	$-0.467166 \cdot 10$
9	$-0.211904 \cdot 10^2$	33	$+0.314767 \cdot 10$	58	$+0.112839 \cdot 10^{18}$	83	$-0.556702 \cdot 10$
10	$-0.219993 \cdot 10^2$	34	$+0.255057 \cdot 10$	59	$+0.942005 \cdot 10^{17}$	84	$-0.663570 \cdot 10$
11	$+0.115623 \cdot 10^2$	35	$+0.200683 \cdot 10$	60	$-0.433278 \cdot 10^2$	85	$+0.268574 \cdot 10^{17}$
12	$+0.620701 \cdot 10^{19}$	36	$+0.149347 \cdot 10$	61	$-0.436236 \cdot 10^2$	86	$+0.290102 \cdot 10^{17}$
13	$-0.241687 \cdot 10^2$	37	$+0.993116 \cdot 10^0$	62	$-0.439175 \cdot 10^2$	87	$-0.506900 \cdot 10^2$
14	$-0.248250 \cdot 10^2$	38	$-0.269315 \cdot 10^{18}$	63	$-0.442090 \cdot 10^2$	88	$-0.509425 \cdot 10^2$
15	$-0.254543 \cdot 10^2$	39	$-0.364558 \cdot 10^2$	64	$-0.620360 \cdot 10^4$	89	$-0.511938 \cdot 10^2$
16	$-0.260597 \cdot 10^2$	40	$-0.368192 \cdot 10^2$	65	$-0.447861 \cdot 10^2$	90	$-0.574440 \cdot 10^2$
17	$-0.266438 \cdot 10^2$	41	$-0.371783 \cdot 10^2$	66	$-0.450717 \cdot 10^2$	91	$-0.516937 \cdot 10^2$
18	$-0.272085 \cdot 10^2$	42	$-0.375329 \cdot 10^2$	67	$-0.453553 \cdot 10^2$	92	$-0.519413 \cdot 10^2$
19	$+0.177196 \cdot 10^{19}$	43	$-0.378833 \cdot 10^2$	68	$-0.456371 \cdot 10^2$	93	$-0.521881 \cdot 10^2$
20	$-0.215973 \cdot 10$	44	$-0.382296 \cdot 10^2$	69	$+0.153371 \cdot 10$	94	$-0.106654 \cdot 10^{18}$
21	$-0.365331 \cdot 10$	45	$-0.385721 \cdot 10^2$	70	$+0.116743 \cdot 10$	95	$-0.106654 \cdot 10^{17}$
22	$-0.595909 \cdot 10$	46	$-0.389108 \cdot 10^2$	71	$+0.802078 \cdot 10^0$	96	$-0.368272 \cdot 10^{17}$
23	$-0.297957 \cdot 10^2$	47	$-0.323855 \cdot 10^{18}$	72	$+0.433747 \cdot 10^0$	97	$+0.205980 \cdot 10^2$
24	$-0.302743 \cdot 10^2$	48	$-0.116973 \cdot 10^2$	73	$+0.580893 \cdot 10^{-1}$	98	$+0.167662 \cdot 10^2$
25	$-0.307410 \cdot 10^2$	49	$-0.176349 \cdot 10^2$	74	$-0.329192 \cdot 10^0$	99	$+0.141366 \cdot 10^2$
		50	$-0.318810 \cdot 10^2$	75	$-0.733158 \cdot 10^0$	100	$+0.122044 \cdot 10^2$

Table 1. The numerical values of the scattering length a given by Eq. (6) for $Z=2$ to $Z=100$.

⁴ A. MESSIAH, Mécanique Quantique, Dunod, Paris 1959, tome 1, p. 347.

⁵ R. B. LEVY and J. B. KELLER, J. Math. Phys. 4, 54 [1963].

Table 2. The numerical values of the total cross-section σ given by Eq. (15) as a function of k for several Z -values.

k	$Z = 60$	$Z = 62$	$Z = 65$	$Z = 66$	$Z = 68$	$Z = 70$	$Z = 74$	$Z = 78$
0.01	0.17301 · 10 ⁵	0.17753 · 10 ⁵	0.18427 · 10 ⁵	0.18651 · 10 ⁵	0.19098 · 10 ⁵	0.13983 · 10 ²	0.85605 · 10	0.41659 · 10 ²
0.02	0.73909 · 10 ⁴	0.75771 · 10 ⁴	0.78541 · 10 ⁴	0.79459 · 10 ⁴	0.81286 · 10 ⁴	0.69456 · 10 ¹	0.23497 · 10	0.17480 · 10 ²
0.03	0.61467 · 10 ³	0.63208 · 10 ³	0.65810 · 10 ³	0.66676 · 10 ³	0.68402 · 10 ³	0.99725 · 10	0.11248 · 10 ⁻¹	0.89752 · 10
0.04	0.27560 · 10 ⁴	0.28190 · 10 ⁴	0.29124 · 10 ⁴	0.29432 · 10 ⁴	0.30046 · 10 ⁴	0.11658 · 10 ¹	0.67457 · 10	0.94958 · 10 ¹
0.05	0.35894 · 10 ⁴	0.34575 · 10 ⁴	0.32575 · 10 ⁴	0.34035 · 10 ⁴	0.30564 · 10 ⁴	0.12491 · 10 ²	0.26992 · 10 ¹	0.60472 · 10 ²
0.06	0.31171 · 10 ⁴	0.32347 · 10 ⁴	0.33697 · 10 ⁴	0.34035 · 10 ⁴	0.34554 · 10 ⁴	0.39790 · 10 ²	0.65362 · 10 ¹	0.16865 · 10 ³
0.07	0.21499 · 10 ⁴	0.23209 · 10 ⁴	0.24952 · 10 ⁴	0.25299 · 10 ⁴	0.25635 · 10 ⁴	0.87208 · 10 ²	0.12603 · 10 ²	0.34142 · 10 ³
0.08	0.16871 · 10 ⁴	0.14471 · 10 ⁴	0.10212 · 10 ⁴	0.87524 · 10 ³	0.59584 · 10 ³	0.15738 · 10 ³	0.21269 · 10 ²	0.56919 · 10 ³
0.09	0.41489 · 10 ³	0.74158 · 10 ³	0.12163 · 10 ⁴	0.13413 · 10 ⁴	0.15091 · 10 ⁴	0.25001 · 10 ³	0.32838 · 10 ²	0.81280 · 10 ³
0.10	0.14157 · 10 ²	0.19557 · 10 ³	0.70468 · 10 ³	0.87966 · 10 ³	0.11521 · 10 ⁴	0.35999 · 10 ³	0.47520 · 10 ²	0.99597 · 10 ³
0.11	0.41048 · 10 ³	0.80091 · 10 ³	0.10321 · 10 ⁴	0.96524 · 10 ³	0.66307 · 10 ³	0.47540 · 10 ³	0.65395 · 10 ²	0.10198 · 10 ⁴
0.12	0.49126 · 10 ³	0.10218 · 10 ³	0.12391 · 10 ³	0.30129 · 10 ³	0.69806 · 10 ³	0.57642 · 10 ³	0.86372 · 10 ²	0.81737 · 10 ³
0.13	0.69579 · 10 ³	0.30396 · 10 ³	0.35726 · 10 ²	0.18459 · 10 ³	0.60072 · 10 ³	0.63701 · 10 ³	0.11014 · 10 ³	0.43813 · 10 ³
0.14	0.26677 · 10 ³	0.20036 · 10 ¹	0.54413 · 10 ³	0.64044 · 10 ³	0.37939 · 10 ³	0.63101 · 10 ³	0.13611 · 10 ³	0.88626 · 10 ²
0.15	0.39721 · 10 ³	0.49616 · 10 ³	0.64507 · 10 ¹	0.15125 · 10 ³	0.54562 · 10 ³	0.54345 · 10 ³	0.16338 · 10 ³	0.15375 · 10 ²
0.16	0.18651 · 10 ³	0.47726 · 10 ³	0.15525 · 10 ²	0.20311 · 10 ³	0.47871 · 10 ³	0.38422 · 10 ³	0.19072 · 10 ³	0.23696 · 10 ³
0.17	0.42564 · 10 ³	0.86354 · 10 ²	0.42027 · 10 ³	0.36137 · 10 ³	0.13794 · 10 ¹	0.19636 · 10 ³	0.21655 · 10 ³	0.42545 · 10 ³
0.18	0.77611 · 10 ¹	0.38767 · 10 ³	0.11937 · 10 ³	0.35814 · 10 ³	0.76387 · 10 ²	0.47864 · 10 ²	0.23902 · 10 ³	0.27778 · 10 ³
0.19	0.84762 · 10 ⁹	0.34751 · 10 ³	0.21956 · 10 ³	0.34021 · 10 ³	0.10396 · 10 ²	0.79492 · 10	0.25613 · 10 ³	0.20695 · 10 ²
0.20	0.17452 · 10 ³	0.50852 · 10 ²	0.15424 · 10 ³	0.58550 · 10 ¹	0.27188 · 10 ³	0.67789 · 10 ²	0.26650 · 10 ³	0.91306 · 10 ³
0.21	0.32101 · 10 ²	0.27219 · 10 ³	0.27323 · 10 ³	0.31182 · 10 ²	0.77120 · 10 ²	0.25506 · 10 ³	0.23671 · 10 ³	0.12961 · 10 ³
0.22	0.54188 · 10 ²	0.23155 · 10 ³	0.15176 · 10 ³	0.20114 · 10 ²	0.22827 · 10 ³	0.20401 · 10 ³	0.26681 · 10 ³	0.80808 · 10 ¹
0.23	0.40188 · 10 ²	0.11373 · 10 ¹	0.94809 · 10 ¹	0.21817 · 10 ³	0.19503 · 10 ³	0.77962 · 10 ²	0.16926 · 10 ³	0.11725 · 10 ³
0.24	0.11494 · 10 ³	0.15911 · 10 ³	0.49809 · 10 ¹	0.13383 · 10 ³	0.14282 · 10 ³	0.98622 · 10	0.12740 · 10 ³	0.16767 · 10 ³
0.25	0.15432 · 10 ³	0.13943 · 10 ³	0.68984 · 10 ²	0.68466 · 10 ²	0.11392 · 10 ³	0.46791 · 10 ²	0.85458 · 10 ²	0.63578 · 10 ²
0.26	0.24598 · 10 ³	0.69257 · 10 ⁻¹	0.14124 · 10 ³	0.91344 · 10	0.59430 · 10 ²	0.14302 · 10 ³	0.48107 · 10 ²	0.41510 · 10 ²
0.27	0.15488 · 10 ³	0.14820 · 10 ³	0.16402 · 10 ³	0.16001 · 10 ³	0.14779 · 10 ³	0.15281 · 10 ³	0.19682 · 10 ²	0.63578 · 10 ²
0.28	0.51211 · 10 ²	0.15940 · 10 ³	0.16001 · 10 ³	0.25966 · 10 ²	0.13217 · 10 ²	0.60236 · 10 ²	0.33860 · 10 ¹	0.11599 · 10 ²
0.29	0.77697 · 10 ²	0.98514 · 10 ²	0.41742 · 10 ²	0.14878 · 10 ³	0.10402 · 10 ³	0.54900 · 10 ²	0.55278 · 10	0.39692 · 10 ¹
0.30	0.13127 · 10 ³	0.23163 · 10 ²	0.13190 · 10 ³	0.38986 · 10 ²	0.89515 · 10 ²	0.12031 · 10 ³	0.10205 · 10 ²	0.12254 · 10 ³
0.31	0.25148 · 10 ²	0.39148 · 10 ²	0.76742 · 10 ²	0.95136 · 10 ¹	0.26923 · 10 ¹	0.54900 · 10 ²	0.29055 · 10 ²	0.54193 · 10 ¹
0.32	0.43321 · 10 ¹	0.68894 · 10 ²	0.10290 · 10 ³	0.55705 · 10 ²	0.89515 · 10 ²	0.12031 · 10 ³	0.52040 · 10 ²	0.94656 · 10 ²
0.33	0.28453 · 10 ¹	0.20149 · 10 ⁷	0.81955 · 10 ²	0.10285 · 10 ³	0.11157 · 10 ³	0.78380 · 10 ²	0.29055 · 10 ²	0.22606 · 10 ²
0.34	0.24885 · 10 ²	0.36524 · 10 ²	0.86387 · 10 ¹	0.33013 · 10 ²	0.10052 · 10 ¹	0.47109 · 10 ¹	0.73332 · 10 ²	0.67509 · 10 ²
0.35	0.99991 · 10 ²	0.62106 · 10 ²	0.88402 · 10 ²	0.99202 · 10 ¹	0.88418 · 10 ¹	0.92374 · 10 ²	0.87632 · 10 ²	0.34118 · 10 ²
0.36	0.10896 · 10 ²	0.88402 · 10 ²	0.37813 · 10 ²	0.49591 · 10 ⁻¹	0.65481 · 10 ²	0.64225 · 10 ²	0.91424 · 10 ²	0.50297 · 10 ²
0.37	0.27543 · 10 ²	0.43670 · 10 ²	0.26965 · 10 ²	0.49591 · 10 ⁻¹	0.61981 · 10 ²	0.28228 · 10 ¹	0.83848 · 10 ²	0.37650 · 10 ²
0.38	0.68541 · 10 ²	0.33469 · 10 ²	0.19284 · 10	0.36577 · 10 ²	0.61981 · 10 ²	0.29266 · 10 ²	0.66915 · 10 ²	0.37650 · 10 ²
0.39	0.74498 · 10 ²	0.53304 · 10 ²	0.45929 · 10 ²	0.78370 · 10 ²	0.18730 · 10 ²	0.77636 · 10 ²	0.44953 · 10 ²	0.41235 · 10 ²
0.40	0.63719 · 10 ²	0.78046 · 10 ²	0.63050 · 10 ²	0.23449 · 10	0.43404 · 10 ²			

for small k -values are given by

$$\delta = -ka - \frac{2k^2 Z \pi}{3A^2 B} - \frac{8Z}{3A^2 B} k^3 \ln|k| + O(k^3). \quad (14)$$

Since a is known, δ can be calculated. Using Eq. (14) for the phase shifts we can calculate the total cross-sections σ for the elastic scattering of low energy electrons within the framework of the Thomas-Fermi theory by means of the well known equation.

$$\sigma = (4\pi/k^2) \sin^2 \delta. \quad (15)$$

In Table 2 we have collected results for σ for certain elements belonging to the same groups in the periodic table.

Table 2 contains the numerical values of the total cross section for several elements. The results show that σ is not a monotonic function of k for small k -values but neither a complicated function of k . σ contains some maxima and minima which means it has an oscillatory character of low energy scattering of electrons by atoms in the Thomas-Fermi theory.

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Kinetic Theory for a Dilute Gas of Particles with "Spin"

III. The Influence of Collinear Static and Oscillating Magnetic Fields on the Viscosity

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The Senftleben-Beenakker effect of the viscosity of dilute polyatomic gases is investigated theoretically for the case where an alternating magnetic field parallel to the usual static field is present. The starting point is a set of transport-relaxation equations obtained from the kinetic equation for the one-particle distribution by application of the moment method. The transport-relaxation equations are solved for the viscosity problem and the relevant viscosity coefficients averaged over many periods of the oscillating field are calculated as functions of the frequency of the alternating field and of the magnitudes of both magnetic fields. The importance of the obtained results for the dynamic behaviour of the thermomagnetic gas torque (Scott effect) is discussed.

The transport properties, in particular heat conductivity and viscosity of dilute polyatomic gases, are influenced by an external magnetic field¹ (Senftleben-Beenakker effects). It is the purpose of this paper to present a theoretical investigation of the effect of two collinear static and alternating magnetic fields on the viscosity of a dilute gas of polyatomic molecules. In view of the close connection between the Senftleben-Beenakker effects for the heat conductivity and viscosity and the "thermomagnetic torque effect" observed for rarefied polyatomic gases² (Scott effect), such an analysis is also of importance for recent Scott effect measure-

ments³ involving collinear static and alternating magnetic fields. A theoretical analysis of this "dynamic behaviour" of the thermomagnetic torque has already been presented by the authors⁴.

The Senftleben-Beenakker effects have been studied extensively (both experimentally and theoretically) during the last decade; for an excellent review of the literature see the article by BEENAKKER and McCOURT⁵. Qualitatively, the influence of a magnetic field on the transport properties of polyatomic gases can be understood as follows. In the transport situation, collisions between molecules possessing a nonspherical interaction give rise to

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² G. G. SCOTT, H. W. STURNER, and R. M. WILLIAMSON, *Phys. Rev.* **158**, 117 [1967].

³ G. W. SMITH and G. G. SCOTT, *Phys. Rev. Letters* **20**, 1469 [1968]; *Phys. Rev.* **188**, 433 [1969].

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⁵ J. J. M. BEENAKKER and F. R. McCOURT, *Ann. Rev. Phys. Chem.* **21**, 47 [1970].