

Validity of the Born Approximation as Applied to Electron-Electron Scattering in Metals: Implications for Thermal Conductivity*

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(Received 30 April 1973)

The frequently quoted result that the Born approximation overestimates electron-electron scattering in metals by a factor of 5 is found to be incorrect. We find for the screened Coulomb interaction $V = e^{-k_s r}/r$ that (i) the Born approximation overestimates the scattering cross section and the electron-electron contribution to the thermal resistivity by about a factor of 2; (ii) the cross section and the thermal resistivity are sensitive functions of the screening wave vector k_s ; and (iii) neither the Thomas-Fermi nor the Bohm-Pines screening wave vector yields a thermal resistivity that agrees with recent experiments on the alkali metals. We conclude that knowledge of the appropriate interelectronic potential is considerably more important for calculating transport coefficients than the use of the Born approximation instead of the exact partial wave method.

I. INTRODUCTION

The present paper summarizes the results of an investigation of electron-electron scattering using a screened Coulomb interaction. We have improved upon the frequently quoted¹⁻⁴ result of Abrahams⁵ that the Born approximation overestimates electron-electron scattering in metals by a factor of 5. By including spin and exchange, and calculating phase shifts for $l=0, 1$, and 2 , we find that the appropriate factor (which depends somewhat on the Fermi energy and choice of screening wave vector) is about 2. Since in fact solid-state theory seldom does better than a factor of 2, one need have little reluctance in using the Born approximation in exploratory calculations on the effect of electron-electron scattering in metals.

We have also calculated the electron-electron scattering contribution to the thermal resistivity of free-electron-like metals starting from exact solutions of the Boltzmann equation. The scattering cross section and the thermal resistivity are found to be sensitive functions of the screening wave vector. Neither the Thomas-Fermi nor the Bohm-Pines screening wave vector yield a thermal resistivity that agrees with recent experiments on the alkali metals. For sodium the calculated resistivity is 20% of the experimental values when Thomas-Fermi screening is used, and three times the experimental value for Bohm-Pines screening. This indicates that the calculated resistivity is very sensitive to the type of screening employed. On this basis we suggest that high-temperature resistivity measurements may serve as a critical test of the appropriate interelectronic potential.

Since the transport coefficients are such sensitive functions of the parameters of the potential

(in our case, the screening wave vector), we conclude that the question of the validity of the Born approximation is secondary in importance to knowledge of the interelectronic potential itself.

II. SCATTERING CROSS SECTIONS

We consider the scattering of one electron by the repulsive screened Coulomb potential $V(r)$ of another, where

$$V(r) = e^{-k_s r}/r. \quad (1)$$

Here k_s is the screening wave vector. We use atomic units throughout ($\hbar = m_e = e = 1$).

The incident energy is the total kinetic energy in the center-of-mass system, or, equivalently, it is the kinetic energy of a particle with reduced mass $\mu = \frac{1}{2}$, moving at the relative velocity of the two electrons.⁶ The incident wave vector k is related to the incident energy by $\epsilon = k^2/2\mu = k^2$. In a free-electron-like metal with Fermi energy ϵ_F and Fermi velocity v_F , the relative velocity ranges between 0 and $2v_F$. Thus the ranges of incident energy and wave vector are given by $0 < \epsilon < 2\epsilon_F$ and $0 < k < k_F$, respectively.

The standard formula for the scattering amplitude in the Born approximation is given in Ref. 7, Eq. (38.1). With potential (1) it is

$$f(\Theta) = -\frac{1}{k_s^2 + q^2}, \quad (2)$$

where $f(\Theta)$ is the amplitude for scattering through an angle Θ in the center-of-mass system. The momentum transfer is given by $q = 2k \sin \frac{1}{2}\Theta = 2\sqrt{\epsilon} \sin \frac{1}{2}\Theta$. The scattering amplitude may on the other hand be found exactly by the partial-wave method [Ref. 7, Eq. (19.11)]. The differential

scattering cross section for identical spin- $\frac{1}{2}$ particles is [Ref. 7, Eq. (41.2)]

$$\sigma(\Theta) = [|f(\Theta)|^2 + |f(\pi - \Theta)|^2 - \text{Re}f(\Theta)f^*(\pi - \Theta)] \quad (3)$$

The total scattering cross section σ is obtained by integrating (3) over solid angle. It is

$$\sigma_{\text{Born}} = 2 \left[\frac{4\pi}{k_s^2(k_s^2 + 4k^2)} \right] - \frac{\pi}{k_s^2(k_s^2 + 2k^2)} \ln \left(\frac{k_s^2 + 4k^2}{k_s^2} \right) \quad (4)$$

and

$$\sigma_{\text{exact}} = \left[\sum_{l=0}^{\infty} \sigma_l \right] + 2 \sum_{l \text{ odd}} \sigma_l \quad (5)$$

with the definition

$$\sigma_l = (2l+1)(4\pi/k^2) \sin^2 \delta_l \quad (6)$$

[The quantities in square brackets in Eqs. (3)–(5) are the cross sections for the scattering of non-identical particles that enter, for example, in calculations of spin diffusion.] The phase shifts δ_l must be calculated numerically by integrating the radial Schrödinger equation. They depend only on the incident energy $\epsilon = k^2$ and the screening wave vector k_s .

Our object is to compare the cross sections (4) and (5) for various choices of incident energy and screening length. For definiteness and ready comparison with Ref. 5, we consider electron-electron scattering in Na, which, in atomic units, has a mean interelectronic distance $r_s = 3.96$ and a Fermi energy $\epsilon_F = 0.117$.

Apart from the question of the adequacy of an interelectronic potential of the form (1), there remains a considerable arbitrariness in the choice of screening wave vector.⁸ Abrahams used the screening wave vector determined by Pines⁹—the cutoff wave vector of the long-wavelength collective oscillations in the Bohm-Pines theory of the electron gas. For Na, Abrahams used $(k_s)_{\text{BP}} = 0.330$. This screening wave vector is about $2\frac{1}{2}$ times smaller than the one obtained by the Thomas-Fermi method⁸:

$$(k_s)_{\text{TF}} = 0.786 \quad (7)$$

Abrahams calculated only the s -wave scattering cross section σ_0 with the Bohm-Pines screening wave vector at two values of the incident energy, 0 and ϵ_F , and concluded that the Born approximation overestimates the scattering by a factor of 5. We have included the contribution of p and d waves (higher waves are completely negligible). With Abrahams's choice of screening wave vector and at the energy $\epsilon = \epsilon_F$, the contribution of p -wave scattering was found to be even greater than that of s -wave scattering.¹⁰ At larger screening wave vectors the s -wave contribution becomes more dominant for fixed incident energy, as it should be

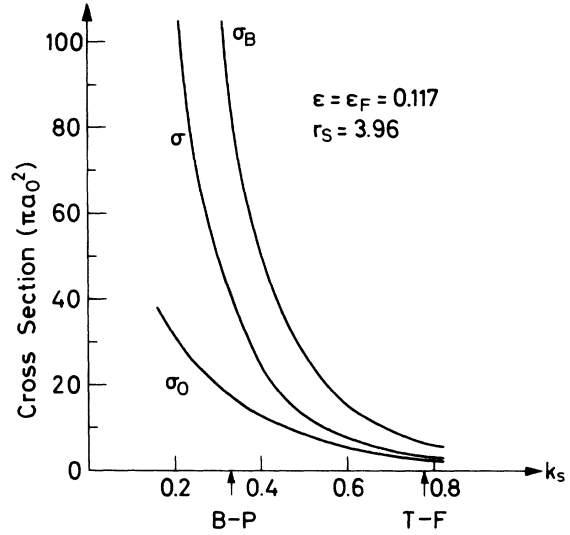


FIG. 1. Electron-electron scattering cross section for a screened Coulomb interaction $V = e^{-k_s r}/r$ plotted vs the screening wave vector k_s at a fixed incident energy $\epsilon = \epsilon_F$ of sodium. The curves labeled σ_0 , σ , and σ_B give the s -wave contribution, the total scattering cross section, and the result of the Born approximation. The values of k_s , r_s , and ϵ_F are in atomic units.

when the range of the potential decreases. The result of varying the screening wave vector and keeping the incident energy fixed (at the Fermi energy) is shown in Fig. 1. Both σ_B and σ depend strongly on k_s and change by more than a factor of 10, when the screening wave vector varies between the Bohm-Pines and Thomas-Fermi values. Also shown is the s -wave contribution σ_0 .¹⁰

In Table I we list σ_0 , σ_1 and σ_2 together with σ , σ_B and their ratio σ_B/σ for three different values of the incident energy using the Thomas-Fermi screening wave vector (7). The ratio σ_B/σ is also plotted versus energy ϵ in Fig. 2. The smaller screening wave vector used by Abrahams gives a ratio that drops rather sharply from its large value at $\epsilon = 0$ when ϵ increases from zero.

TABLE I. Calculated cross section for electron-electron scattering in sodium using a Thomas-Fermi screened Coulomb interaction $(k_s)_{\text{TF}} = 0.786$. The σ_l are the contributions of the l th partial wave, σ is the total cross section, and σ_B is calculated by the Born approximation.

Incident energy	Cross sections (in units of πa_0^2)					
	σ_0	σ_1	σ_2	σ	σ_B	σ_B/σ
0.001 a.u.	4.15	10^{-5}	...	4.15	10.49	2.53
ϵ_F	2.71	0.389	0.003	3.10	6.27	2.02
$2\epsilon_F$	2.00	0.671	0.014	2.69	4.70	1.75

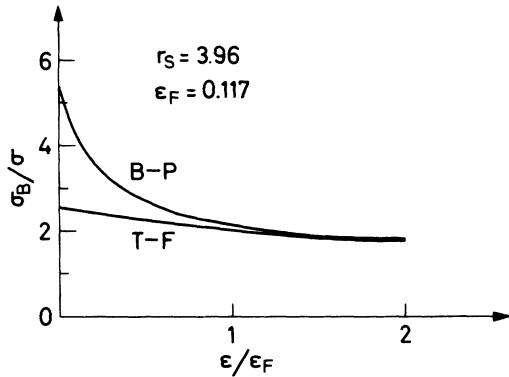


FIG. 2. Ratio of the Born approximation cross section σ_B to the exact cross section σ plotted vs the incident energy. The values of r_s and ϵ_F are those of sodium (atomic units). The curve T-F was obtained with the Thomas-Fermi screening wave vector $(k_s)_{TF}=0.786$, whereas the curve BP used the Bohm-Pines value $(k_s)_{BP}=0.330$.

III. TRANSPORT COEFFICIENTS

Given the dependence of the cross section on the incident energy, what clearly matters in a discussion of the reliability of the Born approximation is what average (over the scattering angle and incident energy) occurs in any physical quantity. For example, in a discussion of particle-particle scattering in degenerate Fermi systems, all transport coefficients are proportional to a characteristic time τ_0 , which is related to an angular average over a collision probability $w(\theta', \phi)$. Specifically,¹¹

$$\frac{1}{\tau_0} = \left(\frac{m^3 (k_F T)^2}{8\pi^4 \hbar^6} \right) \frac{1}{2\pi} \int_0^\pi d\phi \int_0^\pi \sin\theta' d\theta' \frac{w(\theta', \phi)}{\cos \frac{1}{2}\theta'}, \quad (8)$$

where θ' is the angle between the two incoming particles and ϕ is the angle between the plane of incoming particles and that of the outgoing particles. For the degenerate electron gas, where the

scattering particles are all on the Fermi surface, a simple construction¹² leads to the result that ϕ is identical with the center-of-mass scattering angle Θ between the incoming and outgoing relative momenta:

$$\phi = \Theta. \quad (9)$$

Furthermore, a simple calculation of the incident energy in terms of the two incoming momenta leads to the identification

$$\cos\theta' = 1 - \epsilon/\epsilon_F. \quad (10)$$

The connection between the collision probability $w(\theta', \phi)$ and the scattering amplitude $f(\Theta)$ is made explicit in the Appendix.

The electron-electron thermal conductivity κ is¹¹

$$\kappa = \frac{1}{3} C_V v_F^2 \tau_0 (3/2\pi^2) K, \quad (11)$$

where C_V is the specific heat, v_F is the Fermi velocity, and K is a dimensionless quantity, which depends only on the quantity α defined below. In Ref. 11, K was expressed in terms of a rapidly converging series, the sum of which is well approximated by

$$K^{-1} = 1.41 [1 - (\alpha/7.7 - 0.3\alpha)]. \quad (12)$$

For thermal conductivity α is defined by

$$\alpha = 2 \left\langle \frac{w(\theta', \phi)}{\cos \frac{1}{2}\theta'} (1 + 2\cos\theta') \right\rangle \left\langle \frac{w(\theta', \phi)}{\cos \frac{1}{2}\theta'} \right\rangle^{-1} \quad (13)$$

where the brackets denote the same angular integrals as in Eq. (8).

In Table II we summarize the results for the characteristic time τ_0 and the thermal resistivity $W=1/\kappa$ at the Thomas-Fermi and Bohm-Pines screening wave vectors in Na and Cu (we treat Cu as a free-electron-like metal, which only differs from Na with respect to the value of r_s). We observe that for Na, even using a screening wave vector as small as Abrahams did, the use of the Born approximation does not produce a larger discrepancy than a factor of 2.3 in the transport coefficient. The Thomas-Fermi screening wave vec-

TABLE II. Comparison of the exact phase-shift result with the Born approximation for the electron-electron scattering time τ_0 and the thermal resistivity. The screening wave vectors and Fermi energies are those appropriate to sodium ($r_s=3.96$) and copper ($r_s=2.67$).

Screening length	Metal	$T^2\tau_0$ (10^{-6} sec $^\circ K^2$)			W/T (10^{-6} cm/W)		
		Born	Exact	Ratio	Born	Exact	Ratio
Thomas-Fermi	Na	1.1	2.1	1.9	38.0	21.0	1.8
	Cu	2.7	4.5	1.7	4.7	3.0	1.6
Bohm-Pines	Na	0.057	0.14	2.5	710.0	310.0	2.3
	Cu	0.14	0.32	2.3	86.0	40.0	2.1

TABLE III. Electron-electron scattering contribution to the thermal resistivity. Comparison of experiment is made with calculations using a Thomas-Fermi screened Coulomb interaction.

	(W/T) (10^{-6} cm/W)				
	Cu $r_s = 2.67$	Au $r_s = 3.01$	Ag $r_s = 3.02$	Na $r_s = 3.96$	K $r_s = 4.86$
Expt.	4.4	7.3	4.2	100	$\sim 200^a$
Born	5	9	9	38	111
Exact	3^b	5^c	5^c	21^b	60^c

^aPreliminary estimate; see Ref. 15.

^bPhase shifts calculated.

^cUsing interpolation formula (23).

tor results in discrepancies less than a factor of 2. It is also apparent (see Fig. 1) that the magnitude of the cross section (and hence the thermal resistivity), whether calculated exactly or by the Born approximation, depends sensitively on the choice of screening wave vector. Generally we conclude that knowledge of the appropriate screened potential, a problem which we have modeled with our discussion of proper screening wave vectors, is seen to be considerably more important for obtaining the electron-electron cross section in metals and the associated transport coefficients, than the use of the Born approximation instead of the exact partial-wave method. In the Appendix we give an interpolation formula for the thermal resistivity based on our phase-shift analysis.

IV. COMPARISON WITH EXPERIMENT

A measurement of the thermal conductivity of sodium has been recently made by Cook, Van der Meer, and Laubitz.¹⁵ At high temperatures, they observe a small contribution to the thermal resistivity with a linear temperature dependence. They attribute this to electron-electron scattering and estimate that $W/T \approx 100 \times 10^{-6}$ cm/W. This is about 5% of the total thermal resistivity at $T = 300$ °K. We have repeated their procedure for extracting the electron-electron contribution using the data provided in their paper. Using their estimated errors we find that the measured W/T is accurate to $\pm 50\%$.

Our exact calculations in Table II show that neither the Thomas-Fermi nor the Bohm-Pines screened Coulomb potentials yield a W/T that compares well with experiment. We find that a screening wave vector $k_s \approx 0.5$ will reproduce the experimental result for Na.

We have estimated the contribution to the thermal resistivity due to electron-electron umklapp processes in sodium using the results of Lawrence and Wilkins¹⁴ and found it to be negligible. The umklapp processes only affect α slightly, and do

not enter the characteristic time τ_0 . Cook and Laubitz¹⁵ have made high-temperature measurements on potassium and have reported an electron-electron contribution to the thermal resistivity. Similar contributions have been observed in the noble metals and are analyzed by Laubitz.¹⁶ The experimental values in Table III are taken from Laubitz and compared with our estimates.

We might add that interference effects between the several scattering mechanisms present are not able to account for the discrepancy exhibited in Table III. The dominance of the phonon scattering would cause deviations from additivity which are about 25% of the calculated electron-electron thermal resistivity and have the same temperature dependence. This (maximum) deviation from additivity would be accounted for by using the standard variational trial solution, which is linear in the energy variable, rather than the exact one for electron-electron scattering only.¹⁷

We observe that the Thomas-Fermi screening wave vector considerably underestimates the electron-electron scattering in the alkali metals, where we expect free-electron theory to be quite accurate. However, it does give reasonable agreement with the noble metals, where the use of free-electron theory is at best questionable. We note that choosing a new screening wave vector to agree with experiment for the alkalis will spoil the agreement for the noble metals.

We conclude that measurements of the electron-electron contribution to the thermal resistivity constitute a rather severe test of the appropriate interelectronic potential. With that in mind we are currently investigating other models for the interelectronic potential which have vertex corrections built in them and more complicated screening effects than the simple model considered in this paper.

ACKNOWLEDGMENTS

It is a pleasure to thank John Wilkins for relentlessly inspiring this investigation and for numerous discussions, as well as Dr. E. Abrahams for communicating unpublished results. We thank S. Daugård Pedersen for supplying phase shifts for Cu. One of the authors (C.A.K.) appreciates the generous hospitality of Physics Laboratory I of the H.C. Ørsted Institute.

APPENDIX

The transition rate w for the collision

$$\vec{k}_1\sigma_1 + \vec{k}_2\sigma_2 \rightarrow \vec{k}_1'\sigma_1' + \vec{k}_2'\sigma_2' \quad (14)$$

is given by the Golden Rule of perturbation theory, $w(\vec{k}_1\sigma_1, \vec{k}_2\sigma_2; \vec{k}_1'\sigma_1', \vec{k}_2'\sigma_2')$

$$= 2\pi/\hbar \left| V(|\vec{k}_1 - \vec{k}_1'|) \delta_{\sigma_1\sigma_1'} \delta_{\sigma_2\sigma_2'} - V(|\vec{k}_1 - \vec{k}_2'|) \delta_{\sigma_1\sigma_2'} \delta_{\sigma_2\sigma_1'} \right|^2, \quad (15)$$

(leaving out δ functions of momentum and energy). Here

$$V(|\vec{q}|) = \int d\vec{r} e^{i\vec{q}\cdot\vec{r}} V(|\vec{r}|) = (-2\pi\hbar^2/\mu)f(\Theta), \quad (16)$$

with $f(\Theta)$ being the scattering amplitude in the center-of-mass system in the Born approximation.

The natural generalization of the golden-rule result is to use an exact final state in the matrix element rather than plane waves. Schiff [Ref. 7, Eqs. (37.3) and (37.5)] shows that this gives the correct result. We compare the exact result calculated by phase-shift analysis with the Born approximation.

The transition probability needed in Eqs. (8) and (13) is given by $\frac{1}{4}$ of (15) summed over σ_2, σ_1' and σ_2' . The factor of $\frac{1}{4}$ is needed because (8) and (13) implicitly include the sum over final spins. This yields

$$w(\theta', \phi) = \frac{2\pi}{\hbar} \left(\frac{2\pi\hbar^2}{\mu} \right)^2 \frac{\sigma(\Theta)}{2}, \quad (17)$$

where $\sigma(\Theta)$ is given by (3). Using this we find

$$\frac{1}{\tau_0} = \frac{2(k_B T)^2}{\pi\hbar(e^2/a_0)a_0^2} \frac{1}{a_0^2} \left\langle \frac{\sigma(\theta', \phi)}{\cos^{\frac{1}{2}}\theta'} \right\rangle, \quad (18)$$

where

$$\left\langle \frac{\sigma(\theta', \phi)}{\cos^{\frac{1}{2}}\theta'} \right\rangle_{\text{Born}} = \frac{2\sqrt{\beta} a_0^2}{(k_s a_0)^4} \left(\frac{\sqrt{\beta}}{1+\beta} + \sin^{-1}(1+\beta)^{-1/2} - \frac{\beta \cos^{-1}[\beta/(1+\beta)]}{[\beta(1+2\beta)]^{1/2}} \right) \quad (19)$$

and

$$\beta = (k_s/2k_F)^2.$$

The exact result is

$$\left\langle \frac{\sigma(\theta', \phi)}{\cos^{\frac{1}{2}}\theta'} \right\rangle_{\text{exact}} = \frac{a_0^2}{4\pi} \int_0^1 \frac{du}{(1-u)^{1/2}} \Sigma(u), \quad (20)$$

where $u = \epsilon/2\epsilon_F$, and

$$\Sigma(u) = \sigma_0 + \frac{\alpha}{2}\sigma_1 + \frac{55}{32}\sigma_2 + (10\pi/2\epsilon_F\mu)\sin\delta_0\sin\delta_2\cos(\delta_0 - \delta_2).$$

The exact formula must be integrated numerically. Note that phase shifts higher than $l=2$ are neglected. To calculate the thermal conductivity one needs to know the value of α which determines $1/K$ through Eq. (12).

In the Born approximation α is given by a formula only slightly more complicated than (19). The important thing to notice is that α does not change very much as one varies β . For Na the exact values of α for Bohm-Pines and Thomas-Fermi screening are 0.97 and 0.84, respectively, as compared to 1.30 and 1.09 in the Born approximation. Over this range of variation $1/K$ varies with only a few percent [cf. Eq. (12)].

The thermal resistivity $W = 1/\kappa$ may be written as

$$W = \frac{16 m^2 a_0^3}{3 \hbar^3} \gamma_s^3 \left\langle \frac{\sigma(\theta', \phi)}{\cos^{\frac{1}{2}}\theta'} \right\rangle / K T. \quad (21)$$

We write $k_s = A\gamma_s^{1/2}k_F$, which yields the Thomas-Fermi value for $A = (4/9\pi)^{1/6}(4/\pi)^{1/2} = 0.815$. An examination of the expression for W in the Born approximation shows that $(k_s a_0)^4 \langle \sigma(\theta', \phi) / \cos^{\frac{1}{2}}\theta' \rangle$ and K are only weakly dependent on γ_s and A . We have estimated this dependence and constructed the following interpolation formula,

$$W_{\text{Born}} = 1.22 \times 10^{-8} (\gamma_s^{5.34}/A^{3.37}) T \text{ cm }^\circ\text{K/W}, \quad (22)$$

which is good to $\pm 5\%$ for $1.5 < \gamma_s < 6$ and $A_{\text{B-P}} < A < A_{\text{T-F}}$.

The simple power dependence of W on γ_s and A in the Born approximation leads us to write an interpolation formula for the exact phase shift result. We interpolate between $\gamma_s = 2.67$ and 3.96 and between the Bohm-Pines and Thomas-Fermi values of A . This yields

$$W_{\text{exact}} = 1.10 \times 10^{-8} (\gamma_s^{5.04}/A^{3.06}) T \text{ cm }^\circ\text{K/W}, \quad (23)$$

which reproduces our four exact points to $\pm 3\%$. We believe this formula can be used in the range $1.5 < \gamma_s < 6$ to about 10% accuracy.

*Work supported in part by the National Science Foundation under Grant No. GP 27355, and in part by Statens Teknisk-Videnskabelige Fond, Denmark.

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¹²See Figs. 1.4 and 1.5 in David Pines and Philippe Nozières, *The Theory of Quantum Liquids* (Benjamin, New York, 1960), Vol. 1, pp. 58 and 59.

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