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COLLISIONS ACCOMPANIED BY CHARGE EXCHANGE

I. POLUÉKTOV, L. PRESNYAKOV, and I. SOBEL'MAN

P. N. Lebedev Physics Institute, Academy of Sciences U.S.S.R.

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A new formulation of the charge exchange problem is presented, which leads to a system of equations with an Hermitian matrix in the quasi-classical approximation. A general approximate formula for charge exchange probability, which can be applied for arbitrary colliding particle velocities, is obtained. The calculation of the $H^+ + He(1s^2) \rightarrow H(1s) + He^+$ charge exchange cross section on the basis of this formula yields satisfactory results.

1. Collisions of heavy particles, particularly collisions accompanied by charge exchange, can be described in the quasi-classical approximation over a wide energy interval. This approximation consists in assuming the coordinates of the nuclei to be specified functions of the time and not dynamic variables. The problem of charge exchange reduces to a solution of a system of nonstationary perturbation theory equations for the amplitudes of the state probability.

To obtain such equations for a process $A + B^+ \rightarrow A^+ + B$, the total wave function of a system consisting of two ions A^+ and B^+ and an electron is usually written in the form of an expansion in the wave functions of the atoms, formed by attachment of the electron to the ion A^+ (eigenfunctions ψ_i of the atom A) and to the ion B^+ (eigenfunctions φ_m of the atom B) respectively[1,2]. Inasmuch as the ψ and φ are eigenfunctions of different Hamiltonians and are not orthogonal to one another, the resultant system of equations is not Hermitian, and the transition probabilities are not normalized[1]. This apparently is one of the reasons why in the integration of the system the rule has been to confine oneself to the first perturbation theory approximation. Exceptions are the special case of symmetrical resonance and the recently considered[5] charge exchange with a small resonance defect. We note that Demkov[5] calculated the matrix elements of the perturbation in an approximation such that the system was artificially made Hermitian.

In the present paper we present a different formulation of the charge exchange problem[2], leading to a system of equations with Hermitian matrix. We develop an approximate method for integrating this system, analogous to that proposed earlier[6] for the excitation of atoms. A general approximate formula is obtained for the charge-exchange probability, including as limiting cases many of the previously obtained results, particularly in the works of several authors[1,5].

2. We consider first for simplicity the charge exchange occurring when a hydrogen atom collides with a proton. In this case the system consists of two protons, which we denote by A and B, and an electron. The Hamiltonian of the system is of the form[3]

$$H = -{}^1\!/_2\Delta + V(\mathbf{r}_A) + V(\mathbf{r}_B) + W(\mathbf{R}), \tag{1}$$

where r_A and r_B are the radius vectors of the electron relative to the protons A and B; R—distance between protons, which within the framework of the quasi classical method is a specified function of the time:

$$V(\mathbf{r}_A) = -1/r_A, \qquad V(\mathbf{r}_B) = -1/r_B,$$
$$W(\mathbf{R}) = 1/R. \tag{2}$$

Assume that the hydrogen atom consisted prior to the collision of an electron and a proton A. We are interested in a charge exchange process in which the electron goes over to the proton B. We shall henceforth assume the trajectory to be a straight line: $\mathbf{R} = \boldsymbol{\rho} + \mathbf{v}t$, where ρ—impact parameter and $\mathbf{v}$—relative velocity ($\boldsymbol{\rho}\cdot\mathbf{v} = 0$). The reference systems connected with the center of mass and with the centers of atoms A and B are in this case equivalent; it is convenient to choose as the origin the center of the atom B. We represent the total wave function of the system in the form of an expansion in the wave functions φ_m of the atom B,

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[1] More details on the fundamental difficulties connected with such an approach can be found in the papers of Dirac[3] and Sunakawa[4].

[2] We note that an analogous approach is applicable also to other collisions accompanied by particle redistribution.

[3] We employ atomic units throughout.

i.e., in the eigenfunctions of the Hamiltonian H_B:

$$H_B = -{}^1\!/_2\Delta + V(\mathbf{r}_B), \qquad H_B\varphi_m = \varepsilon_m{}^B\varphi_m, \tag{3}$$

$$\Psi(t) = \Big(\sum_m + \int\Big) a_m(t)\,\varphi_m(\mathbf{r}_B)\exp[-i\varepsilon_m^B t], \tag{4}$$

where $(\sum\limits_m + \int)$ denotes summation over the states of the discrete spectrum and integration over the states of the continuous spectrum. The expansion (4) is carried out in a complete system of eigenfunctions of the Hamiltonian (3), and is therefore exact. As $t \to -\infty$ the wave function (4) should describe the hydrogen atom, which consists of an electron and proton A moving with a velocity v:

$$\Psi(t) \to \Psi_{0\mathbf{v}}(t) = \Psi_0(\mathbf{r}_B - \mathbf{R}(t))\exp[i\mathbf{v}\mathbf{r}_B - i(\varepsilon_0{}^A + v^2/2)t], \quad t \to -\infty. \tag{5}$$

Simultaneously

$$a_m(t) \to a_m{}^0(t) = S_{m0}(t)\exp(i\omega_{m0}t), \ \omega_{m0} = \varepsilon_m^B - \varepsilon_0^A, \tag{6}$$

$$S_{m0}(t) = \int \psi_{0\mathbf{v}}\left(\mathbf{r} - \frac{\mathbf{R}}{2}\right) e^{i\mathbf{v}\mathbf{r}}\,\varphi_m^*\left(\mathbf{r} + \frac{\mathbf{R}}{2}\right) d\mathbf{r}. \tag{7}$$

Substituting (4) in the Schrödinger time-dependent equation we obtain the usual system of equations for $a_n(t)$ with Hermitian matrix[4]:

$$i\dot a_m = \Big(\sum_{m'} + \int\Big) H'_{mm'}\exp[i\omega_{mm'}t]\,a_{m'}, \tag{8}$$

$$H'_{mm'} = \int \varphi_m^*(\mathbf{r}_B)\{V(\mathbf{r}_B - \mathbf{R}) + W(\mathbf{R})\}\varphi_{m'}(\mathbf{r}_B)\,d\mathbf{r}_B. \tag{9}$$

The system (8) must be solved with initial conditions (6).

The system (8) can be easily generalized to the case of arbitrary atoms and ions. In this case only (8) will contain potentials averaged over the states of all the internal electrons.

Substituting in the right side of (8) $a_{m'}(t) = a^0_{m'}(t)$ and using the completeness condition for the functions $\varphi_m(r_B)$, we can readily obtain for the charge exchange probability $|a_m(\infty)|^2$ the usual Born formula

$$|a_n(\infty)|^2 = \left|\int_{-\infty}^{\infty} dt\,\langle\varphi_n|V(\mathbf{r}_B - \mathbf{R})|\psi_{0\mathbf{v}}\rangle e^{i\omega_{n0}t}\right|^2. \tag{10}$$

To a certain degree of approximation we can obtain from (8) also a system of two equations for the state probability amplitudes, analogous to that usually considered[1], retaining the hermiticity of the matrix of the equations.

For $m \neq n$ we put

$$a_m(t) = b(t)a_m{}^0(t)[1 - |S_{n0}|^2]^{-1/2}, \qquad a_n(t) = a(t).$$

Substituting these expressions in (8), multiplying each of the equations with $m \neq n$ by $a^{0*}_m(t)[1 - |S_{n0}|^2]^{-1/2}$, and summing all equations with $m \neq n$, we can obtain a system of two equations

$$i\dot a = \tilde V_{nn}a + \tilde V_{n0}e^{i\omega_{n0}t}b, \qquad i\dot b = \tilde V_{0n}e^{i\omega_{0n}t}a + \tilde V_{00}b \tag{11}$$

with initial conditions

$$b(-\infty) = 1, \quad a(-\infty) = a_n{}^0(-\infty) = 0$$

($a^0_n(t) \to 0$ as $|t| \to \infty$, since the discrete-spectrum functions $\varphi_n(\mathbf{r}_B)$ and $\psi_0(\mathbf{r}_B - \mathbf{R})\exp(i\mathbf{v}\cdot\mathbf{r}_B)$ do not overlap as $\mathbf{R}(t) \to \infty$):

$$\tilde V_{nn} = \left\langle\varphi_n^*\left|\frac{1}{|\mathbf{r}_B - \mathbf{R}|}\right|\varphi_n\right\rangle, \tag{12}$$

$$\tilde V_{n0} = [\langle\varphi_n{}^*|r_B{}^{-1}|\psi_{0\mathbf{v}}\rangle - S_{n0}\tilde V_{nn}]/[1 - |S_{n0}|^2]^{1/2}$$

$$\tilde V_{0n} = \tilde V_{n0}{}^*, \tag{13}$$

$$\tilde V_{00} = \{\langle\psi_{0\mathbf{v}}{}^*|r_B{}^{-1}|\psi_{0\mathbf{v}}\rangle - \mathrm{Re}\,[S_{n0}\langle\varphi_n{}^*|r_B{}^{-1}|\psi_{0\mathbf{v}}\rangle - S_{0n}\langle\psi_{0\mathbf{v}}{}^*|r_B{}^{-1}|\varphi_n\rangle] - |S_{n0}|^2\tilde V_{nn}\}[1 - |S_{n0}|^2]^{-1}. \tag{14}$$

It is easy to show that b(t) has the meaning of the state probability amplitude

$$\tilde\Psi(t) = (1 - |S_{n0}|^2)^{-1/2}\{\psi_{0\mathbf{v}} - S_{n0}\varphi_n\}.$$

As $|t| \to \infty$ we have $\tilde\Psi(t) \to \psi_{0\mathbf{v}}$. The functions $\tilde\Psi$ and φ_n are orthogonal for arbitrary t, and therefore $|a|^2 + |b|^2 = 1$. The system of equations (71) and (72) of [1] can also be obtained from (8) if we put (for $m \neq n$) $a_m(t) = b'(t)a^0_m(t)$ and $a_n(t) = a'(t) + b'(t)a^0_n(t)$. As noted above, the matrix of this system is not Hermitian.

3. It is easy to show that the exact solution of the system (11) (a, b) is related to the exact solution of the system (71), (72) from [1] (a′, b′) by

$$a(t) = a'(t) + b'(t)S_{n0}(t),$$

$$b(t) = b'(t)(1 - |S_{n0}|^2). \tag{15}$$

Therefore in those cases when exact solutions can be obtained, for example in symmetrical resonance, the charge exchange probabilities $|a(\infty)|^2$ and $|a'(\infty)|^2$ coincide. On the other hand, in cases when the exact solution cannot be obtained, the system (11), which has a Hermitian matrix, offers certain advantages. In particular, in integrating the system (11) we can use approximate methods previously developed for problems in atomic excitation. We use below a previously derived method, [6] based on the fact that the moduli of the functions a and b, for a system of equations of the type (11) with Hermitian matrix, can be expressed exactly in terms of the phase difference Ω of the functions a and b. The function Ω can be calculated with sufficiently good approximation with the

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[4] As can be seen from (8), the term W(R) introduces only an inessential phase factor in the solution. It will therefore be left out from now on.

aid of the asymptotic methods of the theory of differential equations.

In the general case the nondiagonal matrix elements in (11) are complex:

$$\widetilde{V}_{n0} = Ue^{i\varphi(t)}, \qquad U = |\widetilde{V}_{n0}|. \tag{16}$$

This distinguishes the system (11) from the analogous system of equations in the problem of atomic excitation, where the phase $\varphi(t)$ is equal to zero or is independent of the time. Taking this circumstance into account, the probability of charge exchange can be determined by an approximate formula (compare with formula (15) of the earlier paper[6])

$$w = |a(\infty)|^2 = \Big| \int_{-\infty}^{\infty} U(t) \times \cos\Big(\int_0^t [\omega + \varphi + \widetilde{V}_{nn} - \widetilde{V}_{00} + 4U^2(\tau)]^{1/2} d\tau \Big) dt \Big|^2. \tag{17}$$

It is assumed in (17) that $U(t)$ is an even function. If $U(t)$ is odd, then in (17) we must replace cos (...) by sin (...). For concreteness, the function $U(t)$ will be assumed here even. All further results are independent of this assumption. Formula (17) was discussed in detail before [6]. In particular, it was shown that (17) gives correct expressions for w in several limiting cases, for example the Born approximation and the Landau-Zener case[7].

When $\omega + \dot{\varphi} + \widetilde{V}_{nn} - \widetilde{V}_{00} \gg U$, formula (17) goes over into (82) of [1].

It is easy to show that at large R the potential $\widetilde{V}_{n0}$ decreases by const $\cdot\, e^{-\gamma R}$, where $\gamma = (2I_{min})^{1/2}$ and I_{min} is the smallest of the ionization energies Σ_0^A and Σ_n^B. In this case, using the method developed above,[6] we can obtain from (17) (see Appendix I)

$$w = \exp\Big\{-2\sqrt{\Big(\frac{\pi\omega_{n0}}{\gamma v}\Big)^2 + \Big(\frac{\rho\omega_{0n}}{v}\Big)^2}\Big\} \sin^2 \int_{-\infty}^{\infty} U(t)\, dt. \tag{18}$$

When $\omega_{n0} = 0$, formula (18) assumes the same form as the exact formula for the case of symmetrical resonance. The difference consists only in the fact that instead of the expression

$$(V'_{n0} - S_{n0}H'_{nn}) \, / \, (1 - |S_{n0}|^2) \tag{19}$$

(18) contains $U(t)$ from (16).

In the case of a small resonance defect (small ω_{n0}), where we can leave out the term $(\omega_{n0}\rho/v)^2$ under the radical of the exponential in (17), formula (18) yields, accurate to differences of small significance, the same result as formula (11) from [5].

By way of an example we calculate with the aid of (18), with some supplementary simplifications (see Appendix II), the effective cross section of the charge exchange $H^+ + He(1s^2) \rightarrow He^+(1s) + H(1s)$. We use the Slater approximation for the wave function of the 1s electron of He. All the concrete calculations are given in Appendix II. As a result it became possible to obtain in limiting cases of large and small velocities the simple analytic expressions:

$$\sigma(v) = \frac{\pi v^2 e^{-2\pi\omega_{n0}/v}}{2\omega_{n0}{}^2} \Big[\frac{\pi\omega_{n0}}{v} + \frac{1}{2}\Big], \qquad v \to 0, \tag{20}$$

$$\sigma(v) = \frac{128 a^{3/2} \pi}{5v^2(1 + v^2/4)^5}, \qquad a = 1.7, \qquad v \to \infty. \tag{21}$$

In the intermediate region the cross section $\sigma(v)$ was calculated with an electronic computer. The results of the calculations, and also the experimental data, are shown in the figure. As can be seen from this figure, both the numerical calculations and the interpolation of the limiting formulas (19) and (20) into the region of intermediate values give perfectly satisfactory results. The difference between the interpolation and the numerical calculation does not go beyond the limits of the accuracy that can be expected under the assumptions made.

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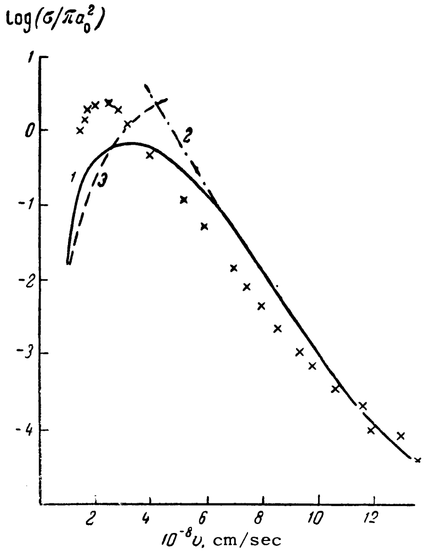
APPENDIX I

When one of the following conditions is satisfied



Effective cross section $\sigma(v)$ of charge exchange $H^+ + He(1s^2) \rightarrow H(1s) + He^+$ (experimental data of[1]): 1 – calculated with formulas (18) and (A II.6); 2 – from formula (21). 3 – from formula (20).

$$|\varphi+\tilde{V}_{nn}-\tilde{V}_{00}|\ll\omega,\qquad |\varphi+\tilde{V}_{nn}-\tilde{V}_{00}|\ll U$$

$$(\omega_{n0}=\omega),$$

the radical in (17) can be replaced by $\omega + 2U$, which differs from the initial radical by not more than a factor $\sqrt{2}$. To calculate the integral

$$|a(\infty)|=\left|\mathrm{Re}\frac{1}{v}\int_{-\infty}^{\infty}U(R)\exp\left\{\frac{i}{v}\left(\int_{0}^{z}2U(R')\,dz'+\omega z\right)\right\}dz\right|,$$

$$R=(\rho^2+z^2)^{1/2} \qquad \text{(AI.1)}$$

we use a contour that is closed in the upper half-plane of the complex variable z, with a cut along the imaginary axis from $i\infty$ to $i\rho$. In calculating the integral (AI.1), we take outside the integral sign the function $\exp(i\omega z/v)$, which is monotonic along the imaginary axis, at the point $\tilde{z}$ in the vicinity of which the derivative of the argument of the exponent in (AI.1) vanishes. The remaining integral is calculated exactly. Recognizing that $U(R) = f(R)\exp(-\gamma R)$, where $f(R)$ is generally speaking a power-law function, we can verify that the points z form along the imaginary axis a sequence

$$\tilde{z}_n=i\sqrt{[\pi(1+2n)]^2/\gamma+\rho^2},\qquad n=0,1,2\ldots \qquad \text{(AI.2)}$$

We take out $\exp(i\omega z/v)$ at the point $\tilde{z}_0$ which gives a maximum contribution to the integral, after which we obtain

$$|a(\infty)|=\exp\left\{-\sqrt{\left(\frac{\pi\omega}{\gamma v}\right)^2+\left(\frac{\omega\rho}{v}\right)^2}\right\}\left|\sin\frac{1}{v}\int_{-\infty}^{\infty}U(R)\,dz\right|. \qquad \text{(AI.3)}$$

For the potential $U = \lambda/\cosh\gamma z$, $\lambda = \text{const}$, Zener and Rosen[8] obtained an exact solution of the initial system of two equations

$$|\ a\infty)\ |=\left[\mathrm{ch}\frac{\pi\omega}{\gamma v}\right]^{-1}\left|\sin\int_{-\infty}^{\infty}\frac{\lambda}{v}[\mathrm{ch}\,\gamma z[^{-1}dz\right|. \qquad \text{(AI.4)*}$$

Formula (AI.3) with $\rho = 0$ and $U = \lambda/\cosh\gamma z$ coincides with (AI.4) if $(\pi\omega/\gamma v) < 1$, and differs from (AI.4) by not more than a factor $\frac{1}{2}$ in the region where $(\pi\omega/\gamma v) \gg 1$ and the result is exponentially small. In the latter case the difference in the pre-exponential factor is due to taking into account only one point z_0 from the sequence z_n, and is of no importance to the results.

APPENDIX II

The wave function of the helium-atom 1s electron has in the Slater approximation the form $\psi(\mathbf{r}) = \pi^{-1/2}a^{3/2}e^{-ar}$, $a = 1.7$; the wave function of the hydrogen-atom 1s electron is $\varphi(\mathbf{r}) = \pi^{-1/2}e^{-r}$. Let us substitute these functions into the matrix elements (19). Leaving out $(1-|S_{n0}|^2)^{-1/2}$ in the denominator of V_{n0} and carrying out the Fourier transformation under the integral sign in (19), we obtain

$$I(\rho,v)=\frac{1}{v}\int_{-\infty}^{\infty}\tilde{V}_{n0}(R)\,dx=I_1(\rho,v)+I_2(\rho,v),\qquad x=vt;$$

$$I_1(\rho,v)=-\frac{16a^{3/2}}{\pi v}\int_{-\infty}^{\infty}dx\int\frac{\exp\{i\mathbf{kR}-ivx/2\}}{(k^2+a^2)((\mathbf{k}-\mathbf{v})^2+1)^2}d\mathbf{k}, \qquad \text{(AII.1)}$$

$$I_2(\rho,v)=\frac{32a^{5/2}}{\pi v}\int_{-\infty}^{\infty}dx\left[\frac{1}{\sqrt{x^2+\rho^2}}-\left[1+\frac{1}{\sqrt{x^2+\rho^2}}\right]e^{-2\sqrt{x^2+\rho^2}}\right.$$
$$\left.\times\int\frac{\exp[i\rho s+iqx]\,ds\,dq\,dl}{(s^2+l^2+(q+v/2)^2+a^2)^2(s^2+l^2+(q-v/2)^2+1)^2}\right. . \qquad \text{(AII.2)}$$

Carrying out the integration with respect to x in (AII.1), we can express I_1 in terms of the Macdonald functions

$$I_1(\rho,v)=-\frac{8a^{3/2}}{v(a^2-1)}\left[\frac{\rho}{\sqrt{1+v^2/4}}K_1\left(\rho\sqrt{1+\frac{v^2}{4}}\right)\right.$$
$$+\frac{2}{(a^2-1)}\left(K_0\left(\rho\sqrt{a^2+\frac{v^2}{4}}\right)\right.$$
$$\left.\left.-K_0\left(\rho\sqrt{1+\frac{v^2}{4}}\right)\right)\right]. \qquad \text{(AII.3)}$$

The multiple integral (AII.2), after integration with respect to x, s, and l, reduces to a single integral of products of Macdonald functions

$$I_2(\rho,v)=\frac{32a^{5/2}}{\pi v}\int_{-\infty}^{\infty}\left[K_0(\rho|q|)-K_0(\rho\sqrt{4+q^2})\right.$$
$$\left.+\frac{2\rho}{\sqrt{4+q^2}}K_1(\rho\sqrt{4+q^2})\right]\left\{\frac{2}{(a^2-1+2vq)^3}\right.$$
$$\times\left[K_0\left(\rho\sqrt{\alpha^2+\left(q+\frac{v}{2}\right)^2}\right)\right.$$
$$\left.-K_0\left(\rho\sqrt{1+\left(q-\frac{v}{2}\right)^2}\right)\right]+\frac{\rho}{2(a^2-1+2vq)^2}$$
$$\times\left[\frac{1}{\sqrt{1+(q-v/2)^2}}K_1\left(\rho\sqrt{1+\left(q-\frac{v}{2}\right)^2}\right)\right.$$
$$\left.\left.+\frac{1}{\sqrt{a^2+(q+v/2)^2}}K_1\left(\rho\sqrt{a^2+\left(q+\frac{v}{2}\right)^2}\right)\right]\right\}dq. \qquad \text{(AII.4)}$$

In accordance with (18), the charge-exchange probability is determined by the formula

$$\sigma(v)=2\pi\int_{0}^{\infty}\rho\,d\rho\,\exp\left\{-2\sqrt{\left(\frac{\pi\omega}{\gamma v}\right)^2+\left(\frac{\rho\omega}{v}\right)^2}\right\}\sin^2\int_{-\infty}^{\infty}U(R)\,dx. \qquad \text{(AII.5)}$$

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*ch = cosh.

Inasmuch as the imaginary part of $\widetilde{V}_{n0}$ is antisymmetrical with respect to time in this case, it drops out in the integration from $-\infty$ to ∞:

$$\int_{-\infty}^{\infty} \widetilde{V}_{n0} dx = \int_{-\infty}^{\infty} U \cos \varphi \, dx.$$

We therefore replace

$$\frac{1}{v} \int_{-\infty}^{\infty} U(R) \, dx$$

by $I(\rho, v)$, which can cause the value to be somewhat lower in the region of the maximum. As a result of such a substitution (AII.5) takes the form

$$\sigma(v) = 2\pi \int_{0}^{\infty} \rho d\rho \exp \left\{ -2 \sqrt{\left(\frac{\pi\omega}{\gamma v}\right)^2 + \left(\frac{\rho\omega}{v}\right)^2} \right\} \sin^2 I(\rho, v). \quad \text{(AII.6)}$$

We note that when $a = 1$ formula (AII.3) goes over into the expression obtained by Brinkman and Kramers, while (AII.4) goes over into the integral given by Murakhver[9].

At small values of v, the quantity $\sin^2 I(\rho, v)$ oscillates strongly, and therefore this factor can be replaced in (AII.6) by $1/2$. For large v, the function $\sigma(v)$ can be expanded in an asymptotic series in reciprocal powers of v. As a result we obtain

$$\sigma(v) \approx \frac{\pi v^2 e^{-2\omega/v}}{2\omega^2} \left[\frac{\pi\omega}{v} + \frac{1}{2} \right], \qquad v \to 0, \quad \text{(AII.7)}$$

$$\sigma(v) \approx \frac{128 a^{3/2} \pi}{5 v^2 (1 + v^2/4)^5}, \qquad v \to \infty. \quad \text{(AII.8)}$$

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