

Theoretical Calculations of Electrical Conductivity In Hydrogen-like Plasma

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Abstract

In this work we calculated electrical resistivity and conductivity for hydrogen like plasma using Ziman like formula. The calculations were carried out for selected values of temperature within the range $10^3 < T < 10^7$ and coupling constant $0.05 < \Gamma < 43.4$ which covers a wide range of plasmas that exist in astrophysics , nuclear fusion and some other physical situations. The calculations depend on previous derivation of the ion-ion static structure factor, effective interaction potential and screening functions, these derivation depends on numerically solving the HNC integral equation with suitable choice of potential and screening or numerical fitting proposed in literature.

The theoretical calculation results of this work were compared with other theoretical methods, quantum molecular dynamics simulation and experimental values when available. All results showed reasonable agreement with experimental and theoretical values, which makes us conclude that methods used in this work suitable for use in further studies and in building numerical and theoretical models for plasma for wide variety of situations and applications.

Keywords: Electrical conductivity, Electrical resistivity, Hydrogen plasma, Ziman formula.

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حسابات نظرية للناقلية الكهربائية للبلازما الشبيهة بالهيدروجين

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الملخص

قمنا في هذا العمل بحساب الناقلية والمقاومية الكهربائيتان للبلازما الشبيهة بالهيدروجين من أجل عدة درجات حرارة ضمن المجال $10^3 < T < 10^7$ وثابت الإقتران للبلازما $0.05 < \Gamma < 43.4$ والتي تغطي مجال واسع من حالات البلازما التي تدرس في الفيزياء الفلكية وتفاعلات الاندماج النووي وبعض الحالات الفيزيائية الأخرى. تعتمد الحسابات على اشتقاقات سابقة لعامل البنية السكوني للإيونات وكمون التأثير المتبادل الفعال وتابع الحجب. وقد اعتمدت هذه الاشتقاقات بشكل رئيسي على الحلول العددية للمعادلة التكاملية HNC أو علاقات تعتمد على هذه النتائج العددية مع اختيار مناسب للكمون و تابع الحجب من النشرات العلمية السابقة. تمت مقارنة نتائج الحسابات النظرية التي حصلنا عليها مع حسابات نظرية أخرى وحسابات المحاكاة بطريقة التحريك الجزيئي الكومومي وبعض القياسات التجريبية، عند توفرها. جميع النتائج المحسوبة في هذا العمل كانت قريبة من القيم التجريبية والطرق النظرية الأخرى، مما يدل على أن الطرق المستخدمة في هذا العمل مناسبة للإستخدام في دراسات مقبلة وفي بناء نماذج نظرية وعددية للبلازما من أجل طيف واسع من الحالات و التطبيقات.

الكلمات المفتاحية: الناقلية الكهربائية، المقاومة الكهربائية، بلازما الهيدروجين، علاقة زيمان.

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1- Introduction:

We can broadly define plasma as a statistical system of mobile charges; plasma has many applications in physics, engineering and in nuclear fusion reactors. Plasma exists in nature in many material states for example in astrophysics plasma exists in surfaces and interior of neutron stars, white dwarfs, the sun and giant planets interior [1,2]. In laboratories examples of condensed plasma are liquid metals and alloys.

Plasma at temperature T is modeled as a number of ions with electric charge Ze and mass M and a negatively charged electrons with mass m . In some cases it is sufficient to consider the plasma consisting of one component to understand its properties, this one component plasma-(OCP) model have one type of charges only embedded in a uniform neutralizing charges (electron and in the background positive ions for example) like Jellium model in liquid metals [3, 4].

To model dense plasma we need to consider multiple species of ions or multi ionic plasmas, we need to define a number of parameters [5, 6].

In multi component plasma the number density of ions and the number density of electrons satisfy the relation:

$$\sum_i Z_i n_i = n_e \quad (1)$$

First for electrons, we define a dimensionless parameter as:

$$r_s = \left(\frac{3}{4\pi n_e} \right)^{1/3} \frac{me^2}{\hbar^2} \quad (2)$$

and r_s is related to the number density of electrons,

The Wigner-Seitz radius of the electrons is given by:

$$a_e = \left(\frac{3}{4\pi n_e} \right)^{1/3} \quad (3)$$

and the Fermi wave number is given by:

$$k_f = (3\pi^2 n_e)^{1/3} = \frac{3.627 \times 10^8 \text{ cm}^{-1}}{r_s} \quad (4)$$

The degree of Fermi degeneracy is:

$$\Theta = \frac{k_B T}{E_F} \quad (5)$$

Θ is related to temperature and Fermi wave number. When $\Theta < 0.1$ the electrons are in the state of complete Fermi degeneracy and thermal

effects are small and quantum effects dominate. When $0.1 \leq \Theta \leq 10$ we have a state where thermal and quantum effects coexist, when $\Theta > 10$ we have a classical state where quantum effects are negligible except for short-range collision.

The coulomb coupling parameter for electrons:

$$\Gamma_e = \frac{e^2}{a_e k_B T} = 2 \left(\frac{4}{9\pi} \right) \frac{r_s}{\Theta} \quad (6)$$

Most classical plasma has $\Gamma \ll 1$, for example in gas discharge plasma Γ is of the order 10^{-3} , in controlled thermonuclear fusion Γ is of the order 10^{-5} and in solar corona Γ is of the order 10^{-7} [1]. In Jovian interior ionic plasma Γ takes value within the range 20-50 and in white dwarf stars from 10 -200.

Wigner-Seitz radius of the ions is given by:

$$a_i = \left(\frac{3Z_i}{4\pi n_e} \right)^{1/3} \quad (7)$$

These parameters are essential in formulating equations to describe plasma.

2- Transport properties in plasma:

The static electrical resistivity is important for characterization of the plasma state. Electric and thermal resistivities in plasma arise from collision and scattering of free electrons with ions in plasma; in order to study this scattering a quantum treatment of the electron-ion interaction is essential to obtain suitable effective potential to describe this interaction. Many previous works have been carried out based on deriving such effective potentials, for example the work of Hansen and McDonald [7], Bernu [8] and Dharma-Wardana [9, 10] to name a few.

Within the Two component plasma TCP – model- the electrical resistivity is given by [1, 2]:

$$\rho_E = 4 \left(\frac{2\pi}{3} \right)^{1/2} \frac{\Gamma_{ei}^{3/2}}{\omega_p} L_E \quad (8)$$

$$\Gamma_{ei} = \frac{Ze^2}{a_i} \quad (9)$$

Where L_E is the generalized coulomb logarithms given by:

$$L_E(\Gamma, \Theta) = \frac{3\sqrt{\pi}\Theta^{3/2}}{4} \int_0^\infty \frac{dk}{k} f_0 \left(\frac{k}{2} \right) \frac{1-G_{ei}(k)}{|\tilde{\epsilon}(k)|^2} S_{ii}(k) \quad (10)$$

Note that f_0 is Fermi distribution and if $G_{ei}=0$ equation (10) becomes the known Ziman formula [1, 3]. In order to obtain generalized coulomb logarithms we need to know ion-ion structure factor $S_{ii}(k)$, local response field G_{ei} and screening function of electron ion interaction $\tilde{\epsilon}(k)$. These two functions can be obtained via computer simulation methods like Monte Carlo and Molecular dynamics or from solving appropriate integral equations of liquid state structure, with a suitable choice of effective potential and screening function. Solutions for the ion-ion structure factor $S_{ii}(k)$, local field correction G_{ei} and thus the generalized coulomb logarithms have been obtained using Hypernetted chain equation (HNC) which proved very effective in the theory of simple liquids, a modified version of HNC using modified convolution approximation (MCA) method [11] is implemented for plasma [12] and a numerical fit have been suggested [1]. Another treatment for HNC equation is implemented taking into account the formation of Rydberg states (RS) in plasma was proposed by Ichimaru [13].

3- Calculations and results:

In this work we calculated the electrical resistivity based on Coulomb logarithm obtained from HNC MCA solution [12], proposed numerical fit given by Ichimaru [12] and the modified solution of HNC including Rydberg states [13]. In order to understand the behavior of electrical resistivity in different regimes, various combination of plasma parameters were chosen to include wide range of plasma parameters which covers classical $\Theta > 1$ and complete degeneracy $\Theta \ll 1$ and correspond to plasma states exist in nature and in laboratory. Results of the electrical resistivity obtained from exact solution of HNC MCA, parameterized numerical fit

to HNC solution and parameterization including Rydberg states using IRS model equation of state for Hydrogen TCP, are given in Table (1) assuming a fully ionized plasma. We can see that results from HNC MCA and RS are close to each other.

Table (1) electrical resistivities calculated in this work based on HNC MCA, numerical fit and RS, units are in Ohm-m

Γ	Θ	n_e	T °K	ρ_E HNC MCA	ρ_E numerical fit	ρ_E with RS
0.05	10	2.14E+24	6.86E+06	1.48510E-09	1.42960E-09	1.53290E-09
0.1	10	2.67E+23	1.71E+06	1.47310E-09	1.41440E-09	1.50430E-09
0.2	10	3.34E+22	4.29E+05	1.79110E-09	1.72600E-09	1.75650E-09
0.3	10	9.90E+21	1.91E+05	2.85380E-09	2.86860E-09	2.96410E-09
0.35	10	6.23E+21	1.40E+05	4.37100E-09	4.87110E-09	4.42810E-09
0.1	5	2.14E+24	3.43E+06	1.13990E-09	1.06660E-09	1.17570E-09
0.2	5	2.67E+23	8.57E+05	1.17470E-09	1.06680E-09	1.16630E-09
0.3	5	7.92E+22	3.81E+05	1.36220E-09	1.21890E-09	1.31850E-09
0.4	5	3.34E+22	2.14E+05	1.76610E-09	1.60750E-09	1.79180E-09
0.5	5	1.71E+22	1.37E+05	2.71900E-09	2.80400E-09	2.93860E-09
0.1	1	2.67E+26	1.71E+07	5.19670E-10	5.31690E-10	6.12890E-10
0.2	1	3.34E+25	4.29E+06	4.40790E-10	4.05150E-10	4.87810E-10
0.3	1	9.90E+24	1.91E+06	4.06710E-10	3.45860E-10	4.30440E-10
0.4	1	4.18E+24	1.07E+06	3.90510E-10	3.12400E-10	3.98730E-10
0.5	1	2.14E+24	6.86E+05	3.84480E-10	2.92690E-10	3.80780E-10
0.6	1	1.24E+24	4.76E+05	3.85400E-10	2.81850E-10	3.72280E-10
0.7	1	7.79E+23	3.50E+05	3.92140E-10	2.77680E-10	3.71910E-10
0.8	1	5.22E+23	2.68E+05	4.04320E-10	2.79290E-10	3.79900E-10
0.9	1	3.67E+23	2.12E+05	4.22640E-10	2.86640E-10	3.97580E-10
1	1	2.67E+23	1.71E+05	4.49710E-10	3.00490E-10	4.27120E-10

1.1	1	2.01E+23	1.42E+05	4.97060E-10	3.22590E-10	4.71450E-10
0.2	0.27151	1.67E+27	1.57E+07	1.25790E-10	1.67580E-10	1.98140E-10
0.6	0.27151	6.18E+25	1.75E+06	9.01270E-11	7.92440E-11	1.00790E-10
1	0.27151	1.34E+25	6.32E+05	7.87110E-11	5.68590E-11	7.73960E-11
1.6	0.27151	3.26E+24	2.47E+05	7.28950E-11	4.42160E-11	6.51430E-11
1.8	0.27151	2.29E+24	1.95E+05	7.26230E-11	4.21760E-11	6.34690E-11
2	0.27151	1.67E+24	1.58E+05	7.31120E-11	4.07690E-11	6.25780E-11
2.4	0.27151	9.66E+23	1.10E+05	7.72440E-11	3.94250E-11	6.28710E-11
2.5	0.27151	8.55E+23	1.01E+05	7.96900E-11	3.93540E-11	6.33770E-11
0.5	0.1	2.14E+27	6.82E+06	2.51030E-11	3.71440E-11	4.10320E-11
0.54301	0.1	1.67E+27	5.79E+06	2.44400E-11	3.47350E-11	3.84760E-11
1	0.1	2.67E+26	1.71E+06	1.99990E-11	2.12160E-11	2.45490E-11
1.629	0.1	6.18E+25	6.46E+05	1.71390E-11	1.45150E-11	1.80500E-11
2	0.1	3.34E+25	4.29E+05	1.61500E-11	1.24730E-11	1.61670E-11
2.7151	0.1	1.34E+25	2.33E+05	1.49600E-11	1.00970E-11	1.40770E-11
3	0.1	9.90E+24	1.91E+05	1.46550E-11	9.47090E-12	1.35570E-11
3.2581	0.1	7.73E+24	1.62E+05	1.44430E-11	9.00510E-12	1.31820E-11
4	0.1	4.18E+24	1.07E+05	1.41010E-11	8.03690E-12	1.24660E-11
4.3441	0.1	3.26E+24	9.09E+04	1.40630E-11	7.72270E-12	1.22680E-11
5	0.1	2.14E+24	6.86E+04	1.41980E-11	7.28790E-12	1.20680E-11
5.4301	0.1	1.67E+24	5.82E+04	1.44760E-11	7.09540E-12	1.20480E-11
5.4301	0.01	1.67E+27	5.79E+05	3.83880E-13	5.81640E-13	5.31240E-13
10	0.01	2.67E+26	1.71E+05	3.13980E-13	3.47330E-13	3.78790E-13
16.29	0.01	6.18E+25	6.46E+04	2.72660E-13	2.34980E-13	3.13400E-13
27.151	0.01	1.34E+25	2.33E+04	2.44890E-13	1.62220E-13	2.79540E-13
30	0.01	9.90E+24	1.91E+04	2.41900E-13	1.52010E-13	2.76290E-13
38.011	0.01	4.87E+24	1.19E+04	2.39990E-13	1.32170E-13	2.72930E-13
43.441	0.01	3.26E+24	9.09E+03	2.43690E-13	1.23560E-13	2.74130E-13

Calculated electrical conductivities ($\sigma = 1/\rho$) obtained taking into account Rydberg stats compared with experimental results for Ar, Xe, Ne and H plasmas [14] are shown in Table (2). We can see that electrical conductivity calculated based on HNC MCA solutions taking into account RS is in good agreement with experiment.

A comparison with other theoretical work is carried out and listed in Table (2): reference [15, 16] calculated electrical conductivity based on t-matrix version of the Ziman theory, reference [17] proposed numerical fit based on Pade-approximation for a wide number of quantum statistical mechanical treatment of fully ionized plasma, reference [6] used Ziman like formula to calculate electrical conductivity, references [18, 19] obtained electrical conductivity within a Virial expansion treatment of a fully ionized plasma, which takes into account many-particle effects and reference [20] calculated conductivity based on relaxation approximation.

Table (2) electrical conductivities calculated in this work compared to experiment and other theoretical work, units are in $(\text{Ohm} - \text{m})^{-1} \times 10^2$

	Γ	θ	n_e	This work	Experiment	Ref [18] and [19]	Ref [8]	Ref [15] and [16]	Ref [20]	Ref [17]	T°K
Ar	0.368	56.9	2.91E+19	198.31	190	226	200	192	216	220	22260
	0.505	33.2	5.67E+19	187.21	155	232	203	204	217	224	20250
	0.604	24.4	8.35E+19	186.25	170	241	209	209	222	232	19270
	0.736	16.7	1.44E+20	212.15	255	272	234	246	244	261	18960
	0.838	13.7	1.77E+20	202.06	245	274	232	241	243	262	17830
Xe	0.564	17.9	2.60E+20	634.33	450	458	442	223	441	453	30120
	0.822	9.24	6.10E+20	734.20	680	544	506	241	491	-	27470
	0.922	7.47	8.18E+20	819.27	740	598	546	262	520	590	27010
	1.153	4.93	1.47E+21	1103	690	767	657	368	607	-	26300
	1.26	4.3	1.64E+21	1093	780	822	660	371	622	797	24890

		4	1								
	1.38	3.6 6	2.08E+2 1	1283	1040	945	728	481	661	-	24600
	1.5	3.3 8	2.05E+2 1	1153	930	950	694	476	630	900	22550
Ne	0.30 3	94. 6	1.14E+1 9	128.9 7	130	174	148	150	165	169	19750
	0.36 7	65	1.97E+1 9	139.4 7	165	187	160	168	179	181	19590
Ar	0.12 8	55 1	7.62E+1 7	82.31	83	96.1	79	-	-	93	19000
	0.16 5	38 5	1.04E+1 8	60.49	79	102	84.3	-	-	102	16360
	0.18	32 4	1.35E+1 8	62.17	76	106	87.1	-	-	105	16340
	0.19	29 1	1.58E+1 8	63.31	64	108	88.9	-	-	107	16320
Xe	0.18 5	40 3	6.45E+1 7	30.39	46.4	70.1	55.8	-	-	69	12430
	0.22 6	27 2	1.15E+1 8	32.08	43.8	75.6	60.1	-	-	75	12340
	0.23 4	25 2	1.30E+1 8	33.11	41.1	76.7	61	-	-	72	12430
	0.19 2	37 1	7.40E+1 7	31.49	48	72.8	58	-	-	77	12540
	0.23 5	25 8	1.33E+1 8	34.94	46.3	78.2	62.3	-	-	-	12710
	0.23 9	23 8	1.45E+1 8	34.74	43.5	79.2	63.1	-	-	-	12610
H	0.17 5	36 4	1.03E+1 8	52.46	62.5	95.4	77.8	-	-	94	15380
	0.16 5	33 7	1.56E+1 8	86.13	91.3	125	104	-	-	124	18690
	0.17	27 6	2.59E+1 8	126.1 8	114.3	156	133	-	-	155	21500

Considering that the experimental error is in the range of 20% to 30% we find a good agreement between our calculations and experiment. However, we cannot expect better correspondence between theory and experiment because of deviations from the Coulomb potential for the electron-ion interaction in rare gases and the occurrence of neutral particles (partial ionization) which inevitably will affect the measured results.

Finally we carried out a comparison of the calculated values of electrical conductivity of Hydrogen plasma to results obtained from applying Quantum molecular dynamics (QMD) [21]. In QMD the optical conductivity $\sigma(\omega)$ is calculated using the Kubo-Greenwood formula within the linear response theory, then the static or dc conductivity is calculated by extrapolation to the limit $\sigma(\omega \rightarrow 0)$. We see from table (3) that QMD results is of the same order as the calculated results in this work with large deviations for some cases, in our opinion these deviations are due to extrapolation to the limit ($\omega \rightarrow 0$) which is outside the calculated values in QMD: as this extrapolation assumes that $\sigma(\omega)$ behaves smoothly near zero and inevitably introduces errors.

Table (3) Comparison of electrical conductivity obtained from this work with those calculated via QMD in units of $(\text{Ohm} - \text{m})^{-1}$, brackets represent power of 10.

Γ	Θ	This work	ref. [21]	Deviation %
20	0.027	7.122[+4]	6.65 [+4]	7
10	0.054	2.289[+4]	6.30 [+4]	63
5	0.109	0.736[+4]	5.00 [+4]	85
2	0.272	0.160[+4]	4.25 [+4]	96
40	0.019	10.92[+4]	2.00 [+4]	446
20	0.038	3.616[+4]	1.85 [+4]	95
10	0.076	1.150[+4]	1.70 [+4]	32
5	0.152	0.384[+4]	1.40 [+4]	72
10	0.109	4.088[+3]	3.50 [+3]	17
8	0.17	1.082[+3]	1.40 [+3]	22

4- Conclusion:

Ziman formula (equation 10 with $G_{ei}=0$) have been shown to give accurate results for electrical conductivity in a number of liquid metals [22,23,24], Ziman like formula used in this work to calculate electrical conductivity in plasmas gave reasonable results which agreed with experiment and other theoretical methods as shown in Table (2). These theoretical methods differ in approximating the electron-ion interaction potential and by treating screening which is important factor in calculating structure factor and in simulations like Molecular Dynamics or Monte Carlo methods [25]. A comparison with electrical conductivity calculated from QMD was made. In our view QMD method is computationally demanding and to calculate the dc conductivity we need to extrapolate from dynamic conductivity which inevitably will introduce some errors [26, 27 and 28].

The current work set the grounds for further investigation of conductivities and other transport properties in plasmas mainly: studying effects of impurities , regions near phase transitions in addition to studying plasma with $Z > 1$ and transport properties dependence on fractional ionization of these plasmas, also electrical resistivity saturation[29].

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