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COMPARISON OF MODELS FOR THE FREE-FREE GAUNT FACTOR AT LOW TEMPERATURES AND FREQUENCIES

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ABSTRACT

We perform calculations for the free-free Gaunt factor at electron and photon energies below 1 Ry in the dipole approximation to the radiation field for a variety of representations of the scattering potential. We consider the static-exchange, static-exchange + model polarization, model exchange, and static models. Within each model, the resulting Schrödinger equation is solved exactly using a linear algebraic prescription. We investigate the rare gas and alkali systems. We find great sensitivity to the models for energies below four electron volts (4 eV). Above this energy, the Gaunt factors for the various models come into better agreement.

I. INTRODUCTION

The free-free absorption or inverse Bremsstrahlung process is important to the proper description of a variety of both laboratory and astrophysical plasmas. The mechanism, which involves the absorption of a photon with the resulting increase in energy of the scattered electron, is mediated by a heavy particle such as an atom or molecule and is described by the following reaction:

$$h\nu + e^-(E) + A \rightarrow e^-(E') + A \quad ,$$

where E(E′) is the initial (final) energy of the colliding electron, A represents a target atom, and $h\nu (= \hbar\omega)$ is the photon energy. The process has been studied using a variety of techniques and approximations[1-18] from simple classical models to elaborate quantum mechanical constructions. In an earlier paper,[13] we investigated the free-free absorption process for various models for photon and electron energies above about ten electron volts (10 eV). We extend this study in this article to a much lower energy regime and to a wider variety of models. In Section II, we give a brief outline of the general theory and of the models employed. We follow this exposition by a description of the results in Section III and reserve Section IV for a few concluding remarks. A more comprehensive description of these calculations is given in Reference 19.

II. THEORETICAL FORMULATIONS

In this section, we derive the basic equations used to calculate the free-free absorption parameters. All our models are based on a full quantum mechanical treatment of the interaction of the photon and electron with the atomic target. We first introduce the basic quantities, such as the free-free Gaunt factor, in terms of the dipole matrix elements and continuum wavefunctions for the colliding electron. We then present a brief description of the methods used to solve for these continuum functions. In all calculations, we employ the dipole approximation to the radiation field.

II.A. GAUNT FACTOR

The free-free absorption coefficient, $a(E,\omega)$, in units of cm^5 is related to a dimensionless quantity, $g(E,\omega)$, called the Gaunt factor, through the expression

$$a(E,\omega) = a_K g(E,\omega) \quad . \tag{1}$$

The scaling term a_K is the Kramer's form of the semiclassical free-free absorption coefficient for an electron interacting with a point charge Ze and is given by[15]

$$a_K = \frac{4\pi\, Z_c{}^2 e^6}{3\sqrt{3}\, m^2{}_c h v \nu^3} \qquad [\mathrm{cm}^5] \quad , \tag{2}$$

where m(v) is the mass (velocity) of the incident electron, e is the unit electron charge, c is the speed of light, h is Planck's constant, and ν is the frequency of the absorbed radiation. For the semiclassical formulation, the quantity Z_c represents the point charge with which the electron interacts. However, for a neutral system, this identification is not appropriate. Since a_K is proportional to $Z_c{}^2$ and $g(E,\omega)$ to $Z_c{}^{-2}$, the dependence on Z_c cancels out of the determination of $a(E,\omega)$. Thus, we may make any choice for Z_c provided we are careful in choosing the same convention when comparing to other calculations.

For most applications, we are interested in the Gaunt factor averaged over a Maxwell-Boltzmann distribution as

$$\bar{g}(T,\omega) = \frac{\int_0^\infty g(E,\omega)\, f(E) dE}{\int_0^\infty f(E) dE} \quad , \tag{3}$$

where

$$f(E)dE = \frac{2}{\pi^{1/2}} (k_B T)^{-3/2} \exp[-E/k_B T] E^{1/2} dE \quad , \tag{4}$$

k_B is the Boltzmann constant, T is the electron temperature, and E is the energy of the electron ($= \frac{1}{2} mv^2$). Upon performing the indicated integrals, we can simplify Eq. (3) to the form

$$\bar{g}(T,\omega) = (k_BT)^{-1} \int_0^\infty g(E,\omega) \exp[-E/k_BT]dE \quad . \tag{5}$$

The integration over energy is usually performed with an n_e-point Gauss-Laguerre quadrature scheme. The averaged Gaunt factor is also related to the absorption coefficient per unit pressure per atom, κ, which is more commonly used in astrophysical models, by:

$$\kappa = C_5 \, Z_c{}^2 \, (\Delta k^2)^{-3} \, \Theta^{3/2} \, \bar{g}(T,\omega) \quad , \quad [\mathrm{cm}^4/\mathrm{dyne}] \tag{6}$$

where Δk^2 is the photon energy in Rydbergs, Θ is given by 5040/T, and C_5 is a constant equal to 2.0991×10^{-28}.

The Gaunt factor in atomic units ($e = \hbar = m = 1$) is expressed in terms of a quantum mechanical matrix element $M^{(1)}$ by

$$g(E,\omega) = \frac{\sqrt{3}(\Delta k^2)^4}{8Z_c^2\pi kk'} M^{(1)} \quad , \tag{7}$$

where $k(k')$ is the wave number ($k = mv/\hbar = 2mE/k^2)^{1/2}$ of the incoming (outgoing) electron. The quantity $M^{(1)}$ is, in turn, related to the dipole matrix element $d_{\ell\ell'}^{(1)}(k|k')$ through a complicated expression involving angular momentum coupling coefficients.[15] The dipole matrix element is given by

$$d_{\ell\ell'}^{(1)} (k|k') = \int_0^\infty f_{k\ell}(r) \, O_1 \, f_{k'\ell'}(r)dr \quad , \tag{8}$$

where

$$O_i = \begin{cases} r & i = 1 \\ d/dr & i = 2 \\ dV/dr & i = 3 \end{cases} ,$$

the continuum wavefunction for an electron scattering from an atomic target (see II.B) is given by $f_{k\ell}(r)$, and $\ell(\ell')$ represents the initial (final) orbital angular momentum of the scattered electron. The first (second) expression for the dipole term is designated the length (velocity) form while the final relationship in terms of the interaction potential is termed the acceleration form. For a local scattering potential, all three expressions should yield the same value for the dipole matrix element. We generally employ the dipole length ($i = 1$) form; a detailed description of the method of calculation is given in Reference 19.

In this report, we shall restrict our attention to elastic scattering from 1) a local potential, 2) a closed-shell target atom or ion, or 3) an atom with a single s-electron outside a closed shell (alkali). Within this restriction, the angular algebra can be greatly simplified, and the quantity $M^{(i)}$ can be expressed as

$$M^{(i)} = \sum_{\ell\ell'}^{\ell m} \ell_{max}\, d_{\ell\ell'}^{(i)}(k|k')^2 \quad , \tag{9}$$

where ℓ_{max} is the maximum value of ℓ and ℓ'. Technically, the sum in Eq. (9) should extend over an infinite range of the orbital angular momentum variables. However, in practical applications, the dipole matrix element decreases rapidly with increasing ℓ, and the sum may be truncated at a finite value ℓ_m.

II.B CONTINUUM SOLUTIONS

In the previous section, we presented the principal expressions used in calculating most free-free absorption parameters of interest. All of these expressions were related to a dipole matrix element $d_{\ell\ell'}^{(i)}$ between the continuum solutions for the incoming and outgoing electrons and a particular operator

$0_{(i)}$. In this section, we give the prescriptions for calculating the scattering wavefunction as well as the various approximations invoked.

For elastic scattering from a target atom, the scattering wavefunction $f_{k\ell}$ is a solution of the following radial Schrödinger equation:

$$Lf_{k\ell}(R) = \int_0^\infty W(R|R') f_{k\ell}(R')\, dR' \quad , \qquad (10)$$

where

$$L = d^2/dR^2 + \ell(\ell + 1)R^{-2} + k^2 \quad , \qquad (11a)$$

and

$$W(R|R') \equiv V(R)\,\delta(R - R') + K(R|R') \quad . \qquad (11b)$$

We have divided the "potential" term W into local and nonlocal parts. The local part usually represents the static or direct interaction while the nonlocal term corresponds to exchange and polarization-correlation effects. The latter interaction arises from virtual excitations to the excited states of the atomic system. In the next subsection (IIC), we shall consider various approximate representations of W.

In all of the derivations of the Gaunt factor in Section II.A, we have assumed the following asymptotic form for the continuum solution:

$$f_{k\ell}(R) \underset{R\to\infty}{\sim} \sin(kR + \ell\pi/2 + \eta_{k\ell}) \quad , \qquad (12)$$

where $\eta_{k\ell}$ is the phase shift. The programs that calculate the solutions employ a slightly different asymptotic behavior

$$f^K_{k\ell}(R) \underset{R\to\infty}{\sim} [\hat{j}_\ell(kR) + \hat{n}_\ell(kR)K]k^{-1/2} \quad , \qquad (13)$$

where $\hat{j}_\ell(\hat{n}_\ell)$ is the Ricatti-Bessel (-Neumann) function of order ℓ, and K is the reactance matrix ($K = \tan(\eta_\ell)$). The reactance matrix form can be converted to the behavior of Eq. (12) by dividing f^K by $[(1 + K^2)/k]^{1/2}$.

We have solved Eq. (10) by a linear algebraic^{20} (LA) scheme. In the LA approach, we convert the differential form of Eq. (10) to an integral equation. This integral formulation is in turn transformed to a set of algebraic equations by introducing a discrete quadrature of n_p points for the integrals and wavefunctions. The resulting set of LA equations can be solved using standard linear systems techniques. The approach is non-iterative and can take full advantage of the vector architecture of the new super computers. In addition, nonlocal terms introduce no additional difficulties.

II.C MODEL POTENTIALS

In this section, we review the various approximations we make to the form of the interaction potential given in Eq. (11b). In general, the "potential" is rather complicated, involving contributions from not only the elastic channels but from all virtual excited states of the compound system. In order to properly represent all these effects, we must employ a multichannel or optical potential formulation^{20} of the scattering problem. We have not performed such calculations in this report although we have compared our various models with the results from more elaborate close-coupling calculations.

1) Static-Exchange (SE)

In the SE approximation, we neglect all virtual excitations but consider the full effect of the Pauli principle on the composite system of ground-state atom and continuum electron. The resulting interaction has the form of Eq. (11b) with both a direct (static) and a nonlocal contribution.^{15,20,21} In this case, the construction of the exchange kernel $K(R|R')$ is confined to orbitals representing the ground state of the target atom or ion.

2) Static-Exchange + Polarization (SEP)

We attempt to enhance the SE model by considering several approximations to the polarization-correlation term, which arises in elastic collisions from the virtual transitions to the excited states of the system. The first two approximations are based on a simple truncation of the long-range form of the polarization potential and have the form

$$V_c(R) = V_p(R)\ [1 - \exp(- (R|R_o)^6)] \tag{14a}$$

and

$$V_c(R) = V_p(R)\ [1 - \exp(- (R|R_o))]^6 \quad , \tag{14b}$$

where

$$V_p(R) \equiv - \frac{\alpha}{2} R^{-4} \quad , \tag{14c}$$

with α the dipole polarizability of the atom. We term the first form SEP1a and the second SEP1b. We adjust the parameter R_o to make the phase shifts agree as close as possible with those of more elaborate calculations.

A second set of models [SEP2] is derived from a free-electron-gas [FEG] representation of the short-range component of the polarization-correlation contribution.[22,23] The approximate potential is given by

$$V_c(R) = \begin{cases} V_{corr}(R) & R < R_o \\ V_p(R) & R > R_o \end{cases} \quad , \tag{15}$$

where V_{corr} is taken from Reference 23. The R_o is the point at which the short- and long-range contributions become equal and is <u>not</u> an adjustable parameter.

The full SEP potential is formed by adding V_c to V_s, the static interaction (see II.C.3), in Eq. (11b) and retaining the exchange contribution.

3) Static

The static or direct interaction potential is given by

$$V_s(\vec{R}) = \int^\infty \rho(\vec{r})|\vec{R} - \vec{r}|^{-1}\, d\vec{r} - Z_N R^{-1} \quad , \tag{16}$$

where Z_N is the nuclear charge and the atomic charge density $\rho(\vec{r})$ has the form

$$\rho(\vec{r}) = \sum_{i=1}^{n_o} n_i |\phi_i(\vec{r})|^2 \quad , \tag{17}$$

with n_o being the number of occupied orbitals, and $n_i(\phi_i)$ being the occupation number (wavefunction) for the i-th bound orbital. For a closed-shell target or for one with a single s-type electron outside a closed shell, Eq. (16) is an exact representation of the static potential. For other atomic targets, this expression represents an "average" of the direct interaction. For the static (S) approximation, we replace V in Eq. (11b) with V_s and neglect K.

4) FEG Exchange

In the two FEG forms, we represent V by V_s and make a local approximation to the exchange term K based on free-electron-gas models.[24] Both forms are proportional to the one-third power of the charge density of Eq. (17) and are distinguished by their asymptotic behavior. The Hara model (HFEGE) contains the ionization energy in its definition of the local momentum while the asymptotically-adjusted expression (AAFEGE) does not.

5) Screened Coulomb and Point Charge

The screened Coulomb or Yukawa potential (Y) has a particularly simple form

$$V_Y(R) = -\frac{Z}{R}\exp[-\lambda R] \tag{18}$$

as does the point charge (PC)

$$V_{PC}(R) = -\frac{Z}{R} \quad . \tag{19}$$

The Y potential is used to study plasma screening effects in a very crude fashion while the PC form is employed to test various schemes for scattering from ions. In both cases V_Y or V_{PC} replace V and exchange is ignored.

We can rank the various models according to accuracy by the following scheme:

1) SEP

2) SE

3) AAFEGE/HFEGE

4) S

5) Y, PC .

The top ranking given the SEP model is only valid in those cases in which we have elaborate close-coupling calculations to test the choice of R_0.

III. RESULTS AND DISCUSSION

In this section, we compare the various model potentials discussed above for the determination of the free-free Gaunt factor. Before presenting the detailed comparison, we first investigate the validity of the various models by comparing with other calculations.

III.A COMPARISON WITH OTHER METHODS

As a first test, we treated atomic hydrogen at infrared frequencies and at temperatures of a few thousand degrees at the SE level. In Table 1, we compare our absorption coefficient, corrected for stimulated emission,[25] with those of John[8] and of Doughty and Frazer.[10] The agreement is quite good over the entire range of temperatures and frequencies. In addition, our results compare well with those of Bell et al,[26] who have probably performed the best calculations to date. Even though these authors include correlation-polarization effects through the solution of multi-channel equations, their results are within 20% of the SE for the range under consideration. In addition, we have obtained similar agreement for He and Ne with other more elaborate calculations[27,28,29] by using the SEP2 model. Finally, in order to check the higher energy regimes, we have found excellent agreement with Green[16] for the screened Coulomb potential. These comparisons indicate that the basic formalism and numerical procedures are being evaluated correctly.

III.B COMPARISON OF MODELS

In this section, we compare the averaged free-free Gaunt factors for the various models for a range of photon energies and electron temperatures extending down from about 10 eV. We make the comparison for several atomic species including the rare gases (He, Ne, Ar) and the alkalis (Li, Na).

In Fig. 1, we make a comparison of the SEP2, SE, AAFEGE, and S models for helium (He). We used the near-Hartree-Fock wavefunction of Clementi[30] to represent the target atom. We used 90 points for the Gauss-Legendre mesh in the LA calculation of the continuum wavefunction and distributed there points in three subregions as follows: 30/0.0 - 1.0/, 30/1.0 - 3.0/, and 30/3.0 - 10.a_0/. To calculate the integral over energy in Eq. (4), we employed a five-point ($n_e = 5$) Gauss-Laguerre quadrature; the sum over partial waves in Eq. (9) was carried to an ℓ_m equal to four (4). In applying the SEP2 polarization-correlation potential, we let α be 1.38 a_0^3 and determined R_0 to be 1.773 a_0.

We observe from Fig. 1 that all models perform reasonably well for He. The S case is approximately a factor of eight too high at the lower energies but comes into good agreement at about 0.5 Ry. The SE and AAFEGE models remain close throughout the entire energy range (0.03 - 1.0 Ry), and both are within fifteen percent or better of the SEP2 result, which is used as a standard.

In Fig. 2, we make a similar comparison for argon (Ar). The parameters employed are as follows: $n_p = 120$, 40/0.0 - 1.0/, 40/1.0 - 3.0/, 40/3.0 - 20./; $n_e = 5$; $\ell_m = 4$; $\alpha = 11.0\ a_0^3$ and $R_0 = 2.9177\ a_0$ (SEP2); and $Z_c = 1$. We note much more striking differences among the models. At the lowest energy (0.03 Ry), the SE and SEP2 models are over a factor of five apart. As the energy rises, the differences between these two cases narrow but still remain near fifteen percent (15%) at 0.3 Ry. The AAFEGE again follows the SE rather closely, the largest difference being about 20%. On the other hand, the S model is in error by over an order of magnitude at the lowest energy and does not reach reasonable agreement with the SEP2 until an energy of about 0.3 Ry or 4 eV. In order to further caution against the cavelier use of models below ¶ 2 eV, we performed additional calculations using the SEP1a model. The cut-off parameter R_0 was adjusted to reproduce the low-energy s- and p-wave scattering results of Thompson,[31] who employed a full treatment of exchange and a model polarization potential. We found an R_0 of 3.0 a_0 gave the best agreement with Thompson. For energies above 0.1 Ry (1.5 eV), the two SEP models agree to better than 15 %; however, at the lowest energy (0.03 Ry ~ 0.4 eV), they differ by almost 40 %. Thus, even two models selected to reproduce the best elastic scattering data for Ar and to properly simulate the electronic interaction can be in substantial disagreement below about one electron volt (1 eV). We observe similar results for neon (Ne).

In Fig. 3, we display the results for Li and observe even larger differences among the various models. The parameters employed are as follows: $n_p = 90$, 30/0.0 - 1.0/, 30/1.0 - 3.0/, and 30/3.0 - 10.0/; $n_e = 5$; $\ell_m = 4$; $\alpha = 164\ a_o^3$ and $R_o = 4.1\ a_o$ (SEP1a); and $Z_c = 1$. As with the previous two systems, we have used the bound orbitals of Clementi.[30] The SEP2 model produces much too strong a polarization potential for e-Li collisions. Instead, we have employed the SEP1a model and adjusted R_o to give the best fit to the parameters of the lowest $^3P^o$ resonance determined from a two-state close-coupling calculation. We again observe differences of almost 50% between the SE and SEP1a models at the lowest energy; above 0.1 Ry, they agree to within 20 %. The AAFEGE case exhibits much greater departs from the SE result for Li than for the rare gases. The results for Na are similar to those for Li and re-enforce the need to employ highly accurate representations of the collision mechanism at energies below a few volts.

IV. CONCLUDING REMARKS

We have calculated averaged free-free Gaunt factors within the dipole approximation to the radiation field for a variety of models to the interaction potential experienced by the continuum electron for photon and electron energies below one Rydberg (1 Ry). We have investigated several atomic species including the rare gases (He, Ne, Ar) and the alkalis (Li, Na). We find great sensitivity of the Gaunt factor to the model employed for energies below four electron volts (4 eV). As the energies rise, the agreement among the various models improves. We judge that for accurate results below 4 eV, elaborate close-coupling or optical potentials schemes must be used. We find that for ions, the sensitivity to the model potential is much less than for the neutrals.

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Table 1. Comparison of Absorption Coefficients for H^- at the SE Level[a,b]

Δk^2	Θ	$\bar{g}_s$	$\bar{g}_t$	$\bar{g}$	κ	κ_E	κ_J	κ_{BKM}
0.05	0.5	4.828(-2)	2.773(-2)	3.287(-2)	1.952	1.060	1.04	
	1.0	3.180(-2)	1.099(-2)	1.620(-2)	2.720	2.152	2.17	2.08
	2.0	2.090(-2)	4.766(-3)	8.799(-3)	4.179	3.997	4.11	3.54
0.10	0.5	7.115(-2)	3.839(-2)	4.658(-2)	0.346	0.274	0.271	
	1.0	5.501(-2)	1.842(-2)	2.757(-2)	0.579	0.554	0.567	0.545
	2.0	4.239(-2)	9.770(-3)	1.792(-2)	1.064	1.062	1.11	0.977
0.20	0.5	1.222(-1)	6.408(-2)	7.860(-2)	0.073	0.070	0.073	
	1.0	1.087(-1)	3.754(-2)	5.532(-2)	0.145	0.145	0.158	
	2.0	9.217(-2)	2.348(-2)	4.065(-2)	0.302	0.302	0.339	

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[a] Nomenclature: Δk^2 is the photon energy in rydbergs; $\Theta = 5040/T$ (kelvins); $\bar{g}_s$ ($\bar{g}_t$) is the averaged Gaunt factor for singlet (triplet) scattering; $\bar{g} = (3\bar{g}_t + \bar{g}_s)/4$; κ is the pressure absorption coefficient; κ_E is this coefficient corrected for stimulated emission, κ_J from Ref. 8 (κ's in units of 10^{-26} cm^4/dyne) and κ_{BKM} from Ref. 26; and $Z_c = 1$.

[b] Parameters: Calculations performed in the LA approximation with $n_p = 90$ and a mesh /0.0 - 1.0/1.0 - 3.0/3.0 - 10.0/ with 30 points per region; $\ell_m = 4$; and $n_e = 5$.

FIGURE CAPTIONS

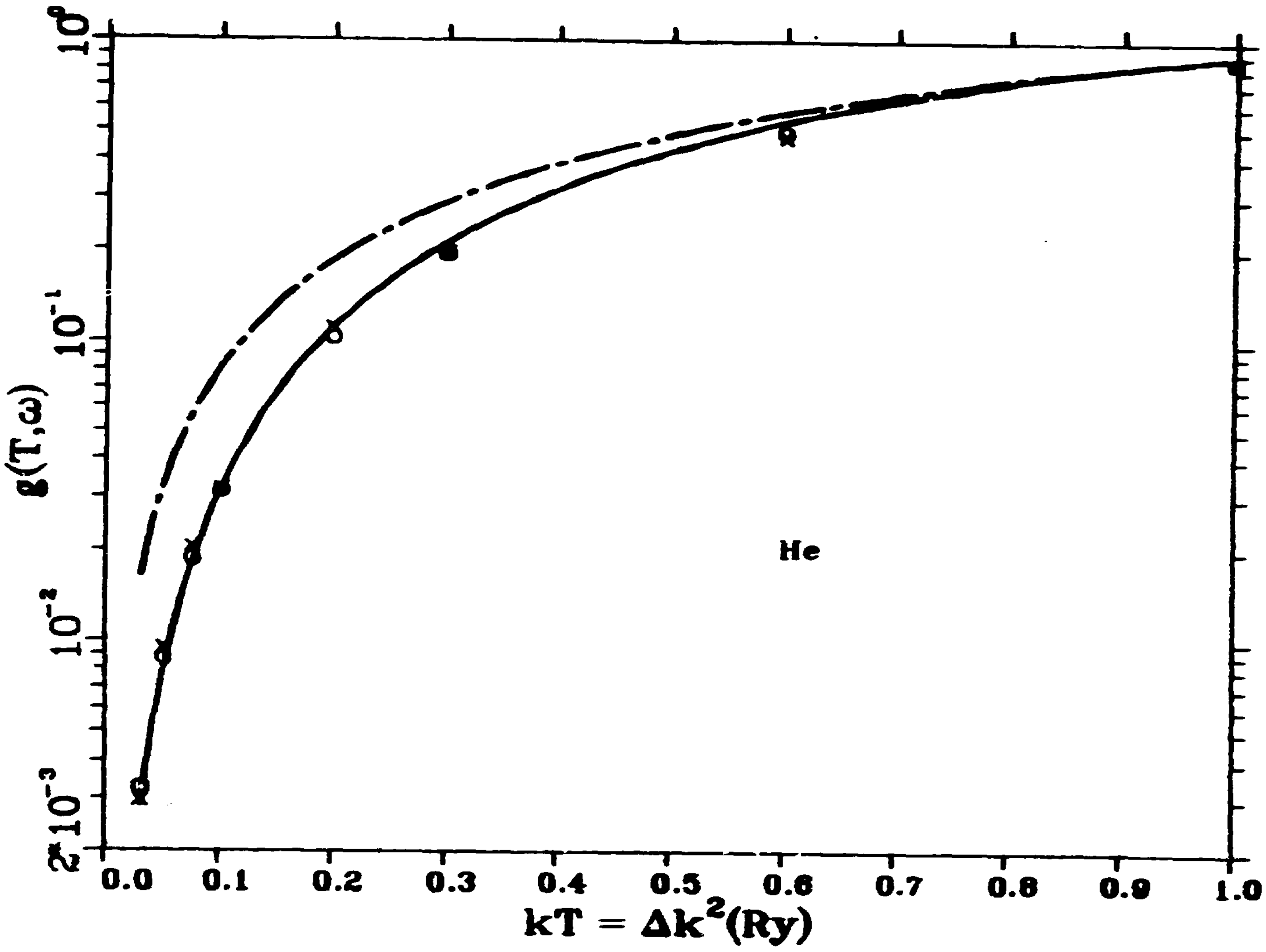
Figure 1: Comparison of Averaged Gaunt Factor $\bar{g}(T,\omega)$ for various models for He.

Nomenclature: Line - SEP2, chain line - S, circle - SE, and cross - AAFEGE

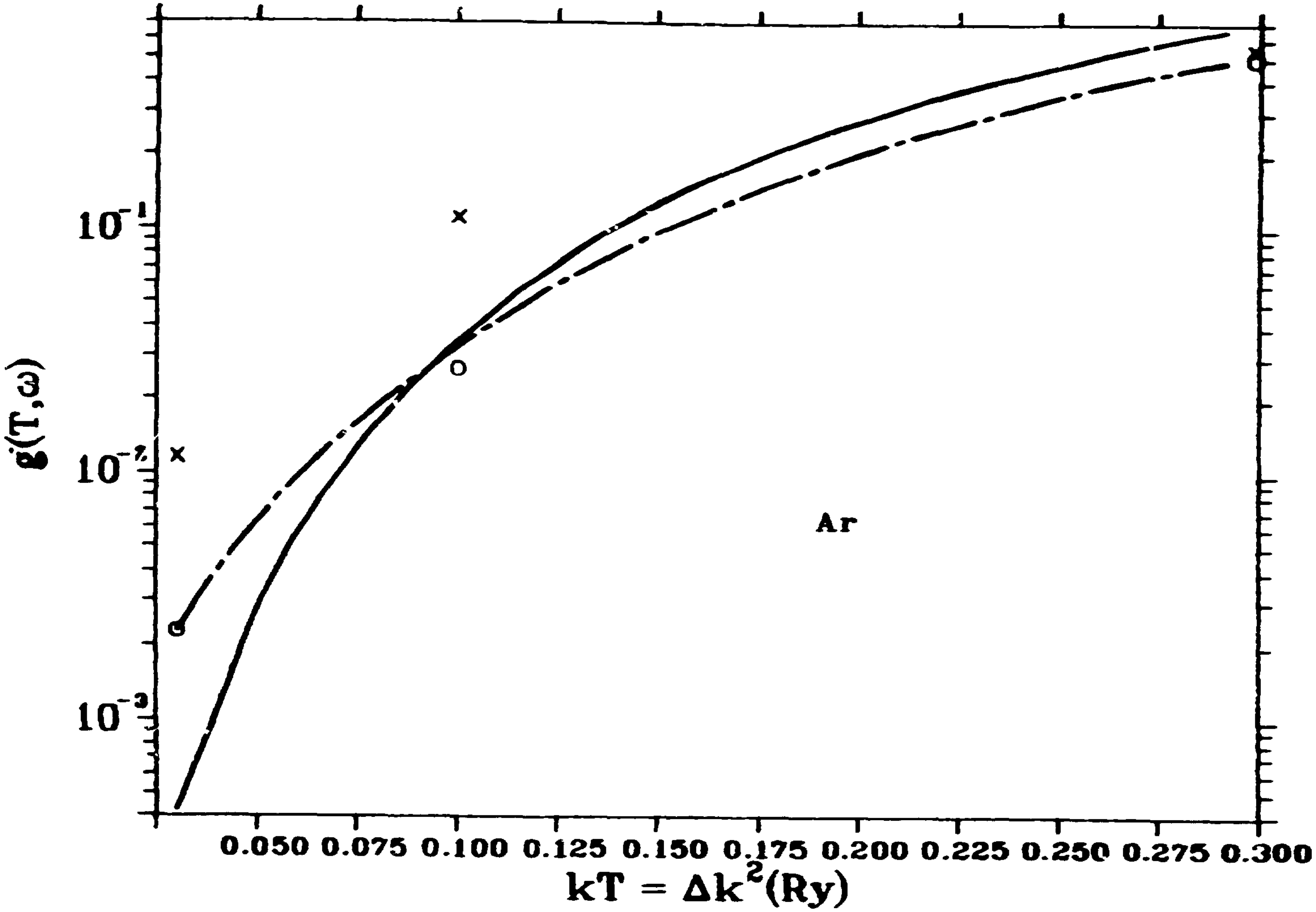
Figure 2: Comparison of $\bar{g}(T,\omega)$ for Various Models for Ar.

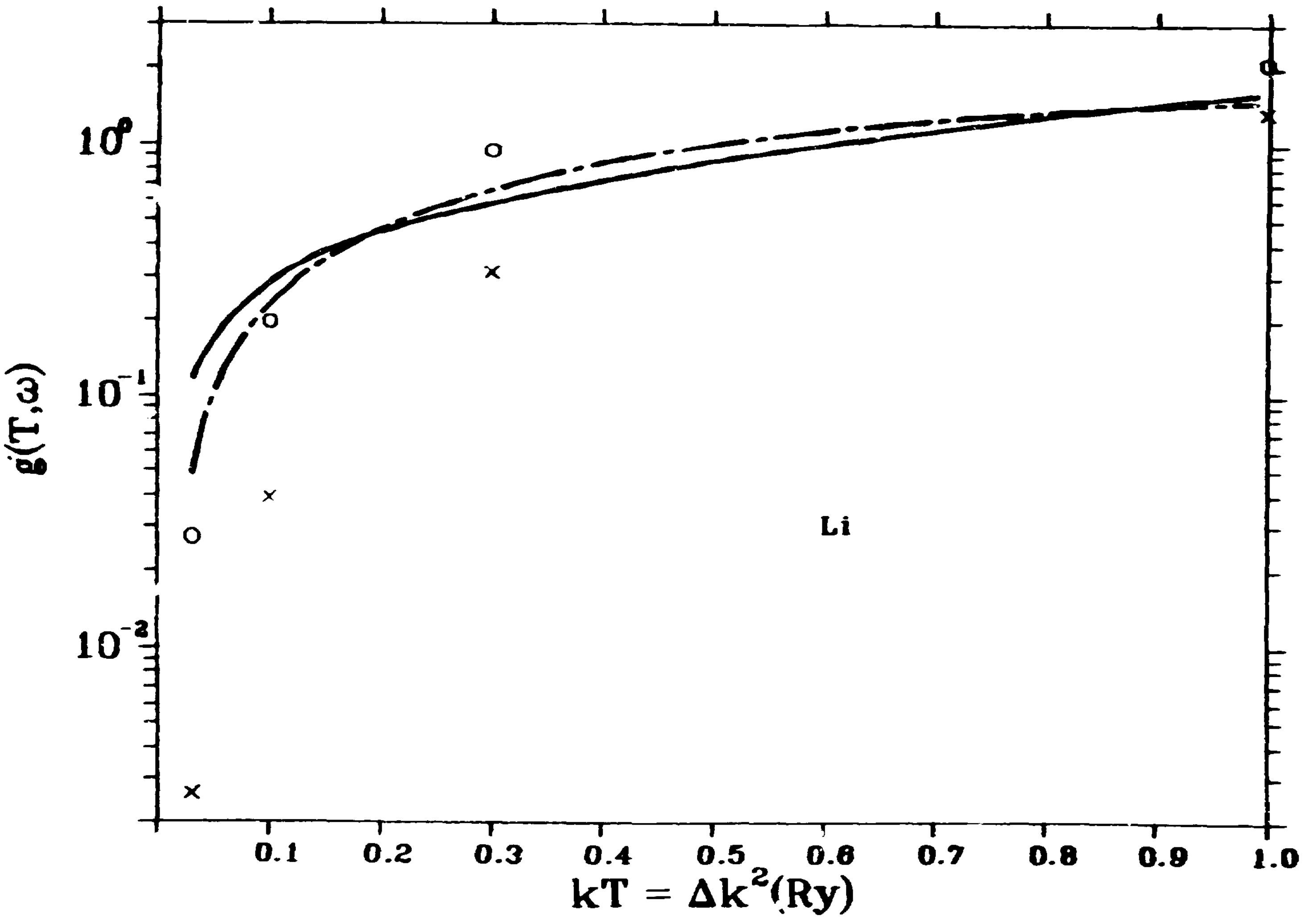
Nomenclature: Line - SEP2, chain line - SE, circle - AAFEGE, and cross - S.

Figure 3: Same as Fig. 2 except for Li; the line represents SEP1b.



10^0
10^{-1}
10^{-2}
10^{-3}
2
g(T,ω)
He
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
$kT = \Delta k^2(Ry)$


10^{-1}
10^{-2}
10^{-3}
$g(T,\omega)$
Ar
0.050
0.075
0.100
0.125
0.150
0.175
0.200
0.225
0.250
0.275
0.300
$kT = \Delta k^2(Ry)$


10^0
10^{-1}
10^{-2}
$g(T,\omega)$
Li
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
$kT = \Delta k^2 (Ry)$