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QUASICLASSICAL REPRESENTATION OF AUTOIONIZATION DECAY RATES IN PARABOLIC COORDINATES

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Abstract

A simple general analytical formula is obtained for autoionization decay rates in parabolic quantum numbers for highly excited atomic states. The formula is applicable for atomic transitions without change of principle quantum numbers ($\Delta n=0$ transitions). A quasiclassical approach for an electron motion in Coulomb field as well as for Clebsh-Gordan coefficient is used for justification of the formula. The results obtained are of universal type applicable for a description of autoionization decay rates in arbitrary ions with complex cores.

Key words: autoionization decay rates, parabolic coordinates, quasiclassical Clebsh-Gordan coefficients

1. Introduction

Autoionization decay rates are important atomic parameters responsible for a number of atomic phenomena in plasmas. The most important applications of these parameters are calculations of dielectronic recombination (DR) rates for multicharged ions in plasmas, see [1] DR plays the main role for ions with complex core in different plasma objects both in laboratory and astrophysical plasmas.

In recent years a numerous papers are devoted to calculations of dielectronic recombination rates in the presence of external electric fields existing in experimental installations (for example, storage rings) or produced by surrounded plasma ions (high density plasmas), see [2]. The strong modifications of DR rates were discovered connected mostly with change of atoms quantization direction in the electric fields (see, for example, [2-4]). The simplest models for these effects are connected with transformation of atomic wave functions from spherical to parabolic basis where the interaction of the atom with external fields is diagonal. Usually this transformation is performed by numerical methods involving a large number of highly excited (Rydberg) atomic states responsible for dielectronic recombination of complex ions. At the same time the contribution of this sates as well as electric field effects can be taken into account in a universal manner on a basis of a quasiclassical approach It is the goal of the paper to obtain a simple universal quasiclassical description for autoionization decay rates in parabolic coordinates which are fast to be applicable for the account of electric fields effects on atomic processes.

To make clear the reasons for applications of quasiclassical methods it is to note that the plasma electrons responsible for a strong dielectronic capture are generally pure classical ones. Really let us consider a multicharged ion with an ion charge Z and complex atomic core having transitions without changing of its principle quantum number n ($\Delta n=0$ transitions). The energy of these transitions is of order of Z atomic units (a u) so the energy $E=mv^2/2$ (v is the electron velocity) of the captured electron must be smaller than Z. At the same time the ionization potential of the ion is of order of Z^2 that is much larger than the electron energy E. These conditions are just the conditions of classical electron motion in the field of the multicharged ion:

$$E < Z << Z^2 \quad or \quad Ze^2 / \eta v >> 1 . \qquad (1)$$

So the electron captured in the field of multicharged ions without change of principal quantum number can be considered on the basis of pure classical mechanics. To do it let us consider matrix elements of electron-electron interaction e^2/r_{12} (r_{12} is the distance between atomic (1) and colliding (2) electrons) in the dipole approximation $\boldsymbol{r}_1\boldsymbol{r}_2/r_2^3$ presenting the wave function of the system as a product of the core wave function and excited electron wave function. Then the matrix element is equal to the product of core matrix element $(r_1)_{if}$ between initial (i) and finite (f) core states and the matrix element of the electric field $\boldsymbol{r}_2 / r_2^3$ produced by the colliding electron on nucleus. The last one can be expressed in terms of electron acceleration $d^2\boldsymbol{r}_2/dt^2$ according the equation of the electron motion in the ion field:

$$\boldsymbol{r}_2 / r_2^3 = Z^1 d^2\boldsymbol{r}_2/dt^2 \qquad (2)$$

According the correspondence principle [5] the matrix elements make a transfer to the corresponding Fourier coefficients. That means that the matrix element from eq.(2) is expressed in terms of Fourier coefficients of its acceleration in the ion Coulomb field well known in classical electrodynamics. The squared of these Fourier coefficients determine intensities of classical electron radiation emission in a Coulomb field, see [6]. Note that classical consideration is applicable even for strong inelastic electron transitions when the change of the electron energy in large as compared with it's initial energy. It is due to the strong electron acceleration in the attractive Coulomb potential being a basis of so called Kramers electrodynamics approach, see [7,8].

The scheme above is used below for quasiclassical consideration of autoionization decay rates.

2. Quasiclassical autoionization decay rates in spherical coordinates

A quasiclassical expression for autoionization decay rate W_A may be obtained by different ways which result in the same formulas. The first way is a direct transition to the classical limit in general formulas for matrix elements of the radius-vector taken with Coulomb wave functions. Note that in the case of Rydberg states ($n>>1$) there is no difference which types of electron transitions (free-bound, bound-bound or free-free) are considered.

The first results were obtained by Zommerfeld [9] for free-free radiative transition in a Coulomb field. He made also a transition to classical limit and obtained quasiclassical formulas for matrix elements as function of scattering angle. With accounting for the relationship between the scattering angle and the electron orbital momentum l one reproduces at fast the total analogues of Kramers classical formulas from the Zommerfeld results. The same results were obtained by Beigman et al [10] by direct calculation of free-bound matrix elements with further transition to the classical limit. The second way is connected with the relationship between the rate W_A and partial electron excitation cross section near threshold [1]:

$$(2l+1)\, g_f W_A(nl) = Z^2 n^{-3} \omega g_i \sigma_{exc}(l) / \pi^2 a_0^2 , \quad (3)$$

where $g_{i,f}$, ω are statistical wages and transition frequency equal to the difference of initial and final energies of the core energy levels.

The electron excitation cross section for $\Delta n=0$ transitions can be also calculated in the frame of pure classical mechanics resulting in the formulae, see [11]:

$$\sigma_{exc}(l) = \frac{8\pi^2}{3}(\eta / mv)^2 \omega_0^2 \left|d_{if}\right|^2 g_f v^{-4}(l+1/2) \times \left\{ \left[H_{iv}^{(1)'}(iv\varepsilon)\right] - (\varepsilon^2 - 1)\varepsilon^{-2}\left[H_{iv}^{(1)}(iv\varepsilon)\right] \right\} \quad (4)$$

where l is the electron orbital momentum, $v = \omega Ze^2/mv^3$, ε is the classical eccentricity of the orbit, d_{if} is the matrix element of dipole momentum of the core, H is the Hankel functions.

The most interesting case responses to the large value of the parameter $v >>1$. For large values of v one obtained finally

$$W_A = \frac{f_{if}}{\pi n^3} lG\left(\frac{\omega_0 M^3}{3Z^2}\right), \quad (5)$$

where f_{ij} is the oscillator strength for the core transition, $M = mv\rho$ is the electron orbital momentum, the function $G(u)$ is equal to :

$$G(u) = u\left[K_{1/3}^2(u) + K_{2/3}^2(u)\right], \quad (6)$$

where $K_{1/3,2/3}$ are McDonald's functions.

The result (5) presents the autoionization decay rate $W_A(n,l)$ in classical approximation. It coincides with the limiting case of quantum mechanical consideration [10] after the standard substitution $l \rightarrow l+1/2$. One can see the sharp decrease of the autoionization decay rate with the increase of the electron orbital momentum l describing by the function G. Taking into account that the essential values of the argument of G-function is never close to zero it is possible for practical using to change the function G by its asymptotic expansion

$$G(u) \approx \pi \exp(-2u) \quad (7)$$

To obtain total autoionization decay rate it is necessary to multiply the eq.(5) by $(2l+1)$ and sum (or integrate) over l. It is more convenient to use the relationship (3) and to express the total autoionization decay rate in terms of total excitation cross section:

$$W_A(n) = 4Z^2 f_{ij}\, g[Z\omega/(2E)^{3/2}] / 3^{1/2} n^3 v^2 , \quad (8)$$

where $g(v)$ is the classical Gaunt-factor for Bremsstruhlung (H are standard Hankel functions):

$$g(v) = \frac{\pi\sqrt{3}}{4} iv H_{iv}^{(1)}(iv\varepsilon) H_{iv}^{(1)'}(iv\varepsilon) \quad (9)$$

Equations (8, 9) can be used for calculations of total autoionization decay rates of the atomic state with principal quantum number n. The precision of the result (9) is the same as the precision of the general relationship (3), the precision of quasiclassical cross sections being very high up to threshold, see [10].

To obtain final result for total autoionozation decay rate one must substitute into (8) the value of the electron energy near threshold $E=mv^2/2=\omega$ that gives

$$W_A(n) = 4Z^2 \left| \; d_{ij} \; \right|^2 g[(Z^2/8\omega)^{1/2}] / 3^{1/2} n^3 \quad (10)$$

The dependence of W_A on Z is practically absent if one takes into account that $d_{ij}^2 \propto Z^2$, the argument of

Gaunt-factor is large if one scales $\omega \propto Z$ that means that the value of g is close to 1 (practically however the argument is not so large).

3. Transformation to parabolic basis

The transformation to parabolic basis may be done also in two ways: 1) calculation of probabilities of an appearance of a specific value of parabolic quantum number in the anglular momenta distribution in Coulomb field and 2) application of the asymptotic representation of Clebsh-Gordan coefficients [12]. Both methods use the specific four dimensional symmetry properties of the Coulomb field. These properties are connected as well known with the additional integral of motion in Coulomb field –Runge-Lentz vector $\boldsymbol{A} = -2e^2\langle \boldsymbol{r} \rangle /3a$ $(a=e^2/2E)$ where $\langle\ \rangle$ means average over the electron motion. The properties of the vector are as follows

$$\boldsymbol{LA}=0\, A^2 + 2EL^2 = 1 \text{ or } n^2\,\varepsilon^2 + l^2 = n^2 \qquad (11)$$

where ε is the eccentricity of the electron orbit and we have substituted quantum numbers l,n instead of orbital momentum and energy.

The evolution of the electron motion can be described in terms of two independent orbital momentums $\boldsymbol{J}_1, \boldsymbol{J}_2$:

$$\boldsymbol{J}_{1,2} = \frac{1}{2}\left[\boldsymbol{L} \pm \left(\frac{m}{a}\right)^{1/2} \boldsymbol{A}\right] \qquad (12)$$

Main properties of the momentums are as follows

$$\begin{aligned} &\hat{\boldsymbol{J}_1^2} = \boldsymbol{J}_2^2 = j(j+1); \\ &(J_1)_z = m_1 = \frac{m + n_2 - n_1}{2}; \\ &(J_2)_z = m_2 = \frac{m + n_1 - n_2}{2}; \\ &L_z = m; \quad \left(\frac{m}{a}\right)^{1/2} A_z = n_2 - n_1 \end{aligned} \qquad (13)$$

The last equation together with eq.(11) describes the connection between projections of vectors $(J_1)_Z$, $(J_2)_Z$ and parabolic $(n_1, n_2, k=n\varepsilon = n_1-n_2)$ and spherical (l,m) quantum numbers. Following conditions are fulfilled in our case of strongly curved classical trajectories corresponding to the formulae (2)

$$m<l<<n \propto j \qquad (14)$$

Equation (13) expresses some limitations on the distribution of projections of these vectors in space. Under conditions (14) one can consider the simplest model when $m=0$. Putting the Z axis along the vector $\boldsymbol{A}$ and X axis along the vector $\boldsymbol{L}$ we can consider a two dimensional model for the evolution of projections J_z and J_x of both vectors $\boldsymbol{J}_1$, $\boldsymbol{J}_2$.

To determine the joint probability $P(l,k,n)$ of appearance of spherical and parabolic quantum numbers l, k let us perform intergration over all phase space of vectors $\boldsymbol{J}_1$, $\boldsymbol{J}_2$ with account for limitations (13). The integrals take the form

$$P(l,k,n) = \int_{-l}^{+l}\int\int\int\int dJ_{1X}\, dJ_{1Z}\, dJ_{2X}\, dJ_{2Z}\, \delta(J_{1Z} + J_{2Z})\, \delta(J_{1Z} - J_{2Z} - k)\, \delta[(J_{1X}^2 + J_{1Z}^2)^{1/2} - j]\, \delta[l - 2(J^2 - J_{1Z}^2)^{1/2}]. \qquad (15)$$

The intergration is performed with the help of properties of δ - functions: $\delta[f(x)] = [df(x)/dx]^{-1}\,\delta(x-x_0)$ $(f(x_0)=0)$ and proper limitations on the domains of variable change.

With account for normalization conditions the result takes the simple form:

$$P(l,k,n,m=0) = 2[(n-1)^2 - k^2]^{-1/2}/\pi \qquad (16)$$

that is the probability of appearance of the parabolic quantum number k doesn't depend on l at all under conditions of small $l<<n$! The probability distribution (15) coincides with the probability of the oscillating variable J_1-J_2 to take a definite value k. It corresponds to a picture of electron motion resulting in the oscillation of orbital momentums $J_{1,2}$ along Z axis with small (neglecting) projections on the X axis.

A close result for the case $m \neq 0$ can be obtained from a consideration of quasiclassical limit of Clebsh-Gordan coefficients. Really the parabolic and spherical quantum numbers are connected by the sum with Clebsh-Gordan coefficients

$$\langle n_1 n_2 m \quad nlm' \rangle = (-1)^{n-1+(2n_2 \pm m - m_1)/2}\, C\left[\frac{n-1}{2}, \frac{n-1}{2}, l; \frac{m + n_2 - n_1}{2}, \frac{m + n_1 - n_2}{2}, m'\right]. \qquad (17)$$

The squared of the coefficients may be considered as a joint probability $P(n,l,k,m)$ of the presence of specific quantum numbers. Making a transit to large values of all quantum numbers [12] and using the conditions (14) determining the domain of present interest one arrives to the following approximation

$$P(n,l,k,m) = C^2[(n-1)/2, (n-1)/2, l; (m-k)/2, (m+k)/2, m] = 2l[(l^2 - l_{min}^2)(l_{max}^2 - l^2)]^{-1/2}/\pi, \quad (18)$$

where

$$l_{min}^2 = \{[(n-1)^2+m^2-k^2] - \{[(n-1)^2+m^2-k^2]^2 - 4(n-1)^2m^2\}^{1/2}\}/2$$
$$l_{max}^2 = \{[(n-1)^2+m^2-k^2] + \{[(n-1)^2+m^2-k^2]^2 - 4(n-1)^2m^2\}^{1/2}\}/2 \quad (18a)$$

or, when $m<<n$

$$l_{min}^2 \approx (n-1)^2 m^2 [(n-1)^2+m^2-k^2]^{-1}$$
$$l_{max}^2 \approx [(n-1)^2+m^2-k^2] = (n-1)^2 m^2 / l_{min}^2 \quad (18b)$$

One can see that when $m=0$ the eq.(18) reduces to the classical eq.(16). The difference between both probability distributions is inside a small domain $[(n-1)-k] \approx m<<n$.

The normalization of $P(n,l,k,m)$ (18) is equal to 1. Really, the integration (18) over l^2 gives the expression

$$J = -\pi \arcsin \left. \frac{-2l^2 + l_{max}^2 + l_{min}^2}{l_{max}^2 + l_{min}^2} \right|_{l_{min}^2}^{l_{max}^2} = 1$$

The parabolic representation of a autoionization decay rate is obtained by multiplication of the rate in spherical basis (5) by the probability (18) and integrating (summing) over l

$$W_A(n, k, m) = \int_{l_{min}}^{l_{max}} dl P(n,l,k,m) W_A(n,l) \quad (19)$$

where l_{min}, l_{max} are defined by eq. (18a) or (18b).

Substituting the expressions (5), (18) for functions $W_A(n,l)$ and $P(n,l,k,m)$ and making a transformation to dimensionless variables $t = l/l_{ef}$, $l_{ef} = (3Z^2/\omega)^{1/3}$ it is possible to obtain:

$$W_A(n, k, m) = \pi^{-1} n^{-3} f_{ij} \; I(n,k,m), \quad (20)$$

where the universal function $I(n,k,m)$ is

$$I(n,k,m) = I(t_{min}, t_{max}) = 2l_{ef}/\pi \int_{t_{min}}^{t_{max}} dt\, t^2 G(t^3) (t^2 - t_{min}^2)^{-1/2} (t_{max}^2 - t^2)^{-1/2} \quad (21)$$

where G was defined by (6) and (7), $t_{min} \approx (n-1)\, m\, [(n-1)^2+m^2-k^2]^{-1/2}$, $t_{max} = (n-1)m/t_{tmin} \approx n$.

Below we will use the approximation (7) for our particular calculations.

One can see that for the case $t_{max} \approx n >> 1$ eq. (21) may be transformed to:

$$I(t_{min}, t_{max}) \approx 2l_{ef}/\pi t_{max} \int_{t_{min}}^{\infty} dt\, t^2 G(t^3) (t^2 - t_{min}^2)^{-1/2}$$
$$\approx 2l_{ef}/t_{max} \int_{t_{min}}^{\infty} dt\, t^2 \exp(-2t^3) (t^2 - t_{min}^2)^{-1/2}$$
$$= I(t_{min})\, 2l_{ef}/t_{max} \quad (22)$$

The universal function $I(x)$ is presented on Fig. 1.

Limiting cases of the function $I(x)$ are as follows:

$$I(x) \approx \begin{cases} \Gamma(2/3)/2^{2/3}3, & x << 1 \\ (\pi/12)^{1/2} x^{1/2} \exp(-2x^3), & x >> 1. \end{cases} \quad (23)$$

The dependences of dimensionless autoionization decay rate $I(n,k,m)(\pi)^{-1}$ from eq. (21) on "electric" quantum number k for different values of magnetic quantum number m are presented on Figs.2-5 for *Li*-like ion ZnXXVIII (Z=30). One can see that the most contribution into k-phase space comes from small values m.

4. Conclusion

The consideration above results in the simple quasiclassical formula (20) for autoionization decay rate in parabolic quantum numbers k,m. It is applicable for the atomic processes accompanied by transitions in atomic cores without change of it's principle quantum number ($\Delta n=0$ transitions). These transitions are responsible for the most contribution to atomic processes in collisions of electrons with complex ions. Just for such processes the conditions (1) for quasiclassical electron motion are provided. The present result makes it possible to calculate autionization decay rates in a simple way for every ions having $\Delta n=0$ transitions in the cores using scaling data for energy levels and oscillator strengths [13].

The results are essential as already pointed for atomic processes in plasmas where external or plasma electric fields provide parabolic quantization of atoms.

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Figure captions

Fig.1 The universal function $I(t_{min})$.

Fig. 2. Distribution of autoionization decay rates over "electric" quantum numbers k at different values of magnetic quantum numbers m for Li-like ion ZnXXVIII at the principal quantum number $n=100$. Here the scale for $I(100,k,10)$ equals to the scale for $I(100,k,0)$ multiplied by 10^1.

Fig. 3. The same as on Fig.2 but for $n=50$. Here the scale for $I(50,k,10)$ equals to the scale for $I(50,k,0)$ multiplied by 10^1.

Fig.4. The same as on Figs.2,3 but for $n=30$: $I(30,k,m)$.

Fig.5. The same as on Figs.2,3,4 but for $n=10$: $I(10,k,m)$.

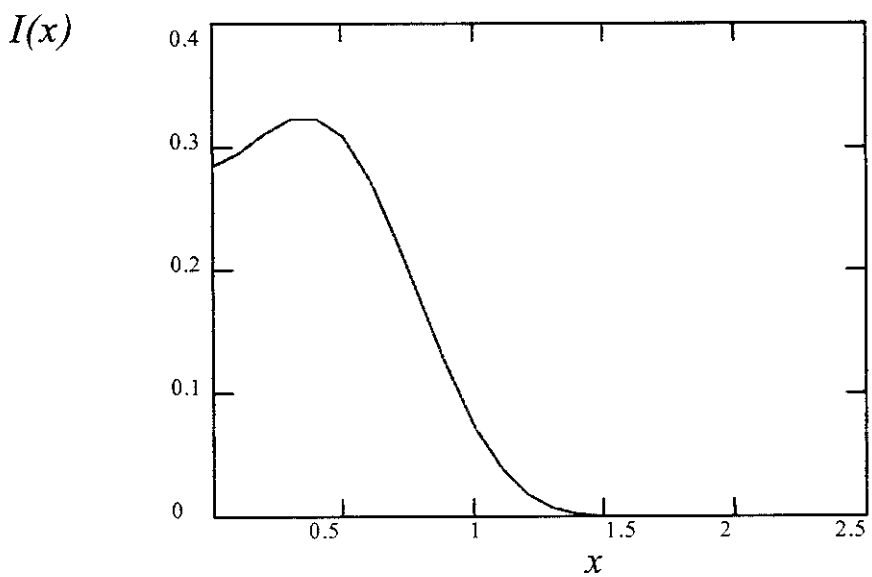

Fig.1

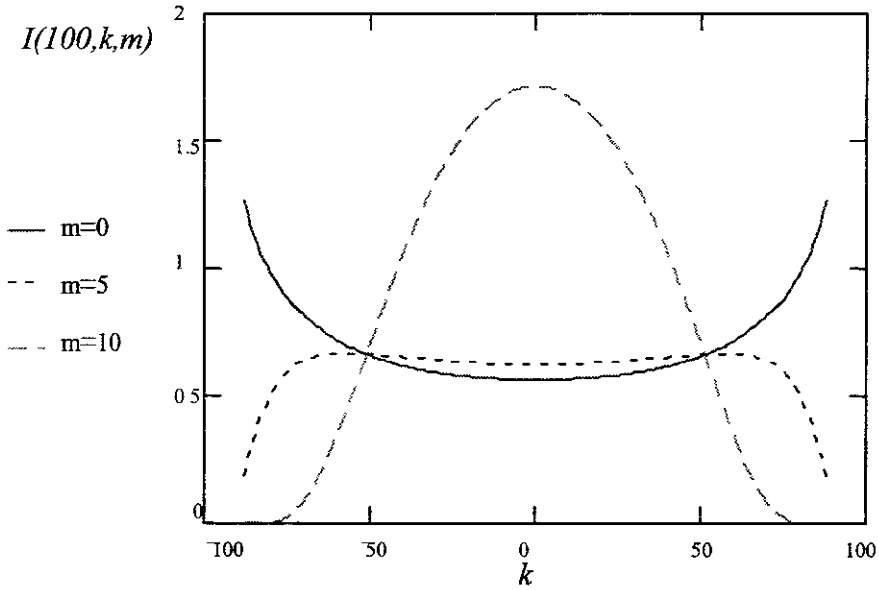
I(100,k,m)
m=0
m=5
m=10
2
1.5
1
0.5
0
-100
-50
0
50
100
k

Fig. 2

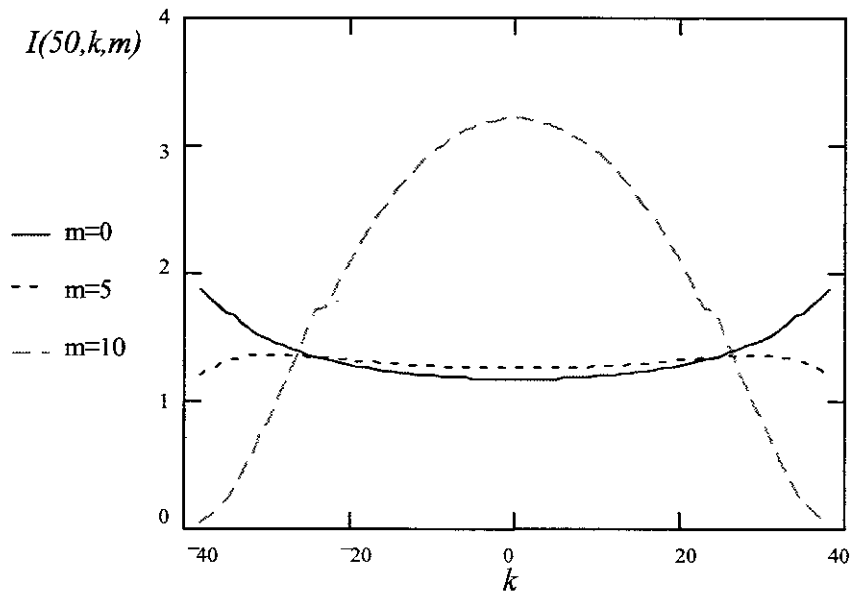
I(50,k,m)
m=0
m=5
m=10
4
3
2
1
0
-40
-20
0
20
40
k

Fig.3

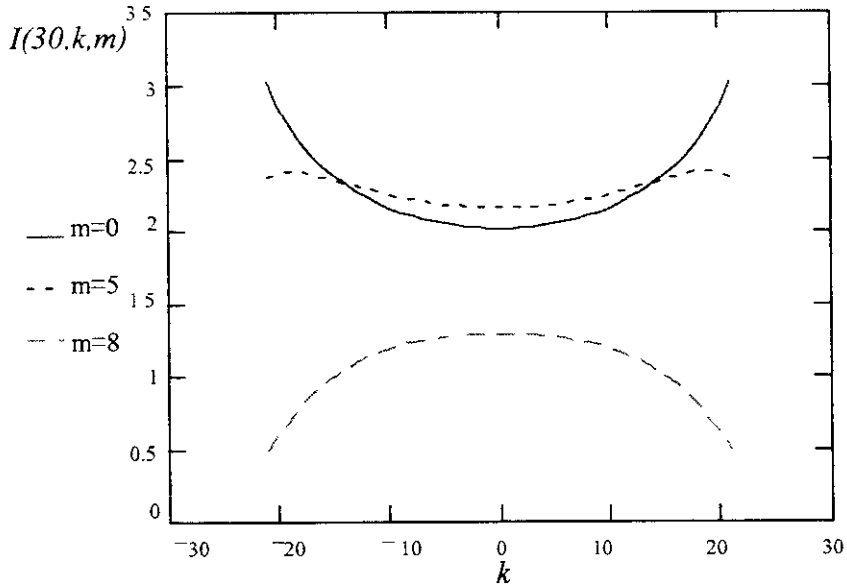
I(30,k,m)
3.5
3
2.5
2
1.5
1
0.5
0
m=0
m=5
m=8
−30
−20
−10
0
10
20
30
k

Fig.4

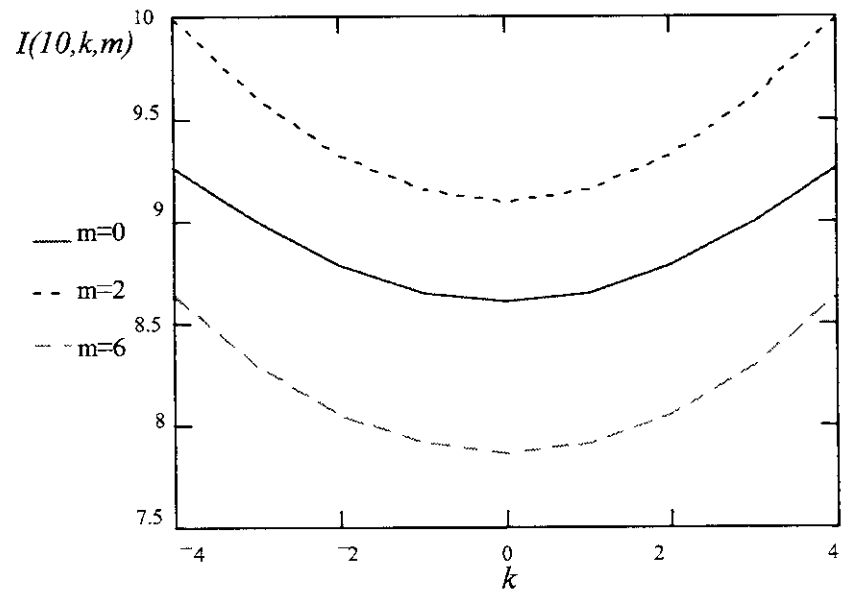
I(10,k,m)
10
9.5
9
8.5
8
7.5
m=0
m=2
m=6
−4
−2
0
2
4
k

Fig. 5

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