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Light scattering by amorphous silicon and amorphous carbon particles at different heliocentric distances

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Abstract. The paper focuses on temperature behaviour of material optical properties, which may play an important role also in dust dynamics. In particular, the study deals with efficiency factors for scattering Q_{sca}, extinction Q_{ext}, and radiation pressure Q_{pr}, and with asymmetry parameter $\langle cos \rangle$. Some constituents of composite particles (like amorphous carbon) may exhibit nonnegligible temperature dependence of the refractive index, and thus certainly change orbital evolution of small interplanetary dust particles. Such temperature effect was unknown until now, and brings a novelty into modelling of dust dynamics.

Spectral and integral optical properties of dust grains are discussed in more detail, and attention is paid to their dependence on heliocentric distance. It is shown that imaginary part of complex refractive index of amorphous silicon and amorphous carbon particles changes markedly with distance from the Sun. Nevertheless, the particles with sizes larger than 1.5 μm behave almost independently of temperature in the outer parts of Earth's orbit. But, the submicron-sized and small micron-sized particles with temperature dependent dielectric function are evolutionary affected when they move at trajectories with close approaches to the Sun (i.e. when the perihelion distance of the orbit is less than $\approx$ 1 AU). The optical properties of particles with sizes less than 1 μm react on temperature variation quite efficiently.

Key words: dielectric function – light scattering – dust dynamics

1. Introduction

In general, the orbital evolution of cosmic dust particles is driven by various forces. Besides gravitational forces, also nongravitational ones can be important. The small sub-micrometer sized and micrometer-sized grains undergo significant dynamical changes especially due to mutual action of electromagnetic radiation field and Lorentz force (LF) - acting exclusively on charged particles. The evolution of non-charged spherical dust particles is known already for seven decades as the Poynting-Robertson (P-R) effect (Robertson, 1937; as for the most comprehensive treatment see Klačka 2004). P-R effect causes the spiraling of the particles towards the Sun and is usually employed for modelling the zodiacal cloud (Ishimoto, 2000; Leinert et al., 1983), dust produced by comets (Sykes et al., 1986; Reach et al., 2000) and asteroids (Dermott et al., 2000), dust near mean-motion resonances with planets (Jackson and Zook, 1989; Liou and Zook, 1997), dust in planetary rings, and also dust in exo-solar systems (Backman and Paresce, 1993; Kohler and Mann, 2002). Contrary to bigger meteoroids, which are controlled by gravitational interactions, the dynamics of micron-sized particles is dominated by electromagnetic radiation besides gravitation. Such small grains do not collide frequently and rather sublimate before they can be destroyed by mutual collisions.

Optical properties of small cosmic grains are one of the most important quantities affecting the dynamics of each individual dust particle. Variable chemical composition of cosmic dust particles and abundances of specific materials are responsible for different optical responses of dust particles to an incident electromagnetic radiation field. The reason is that the efficiency factor for radiation pressure depends on dielectric function, which changes with material configuration inside the particle. The real composition of the cosmic dust particles is given by their origin and evolution in the space. The cosmic abundance of elements making highly refractory grains (mainly Mg, Si, and Fe) is for instance lower than the abundance of C, N, and O, which form relatively volatile ices (Salpeter, 1977). As for the solar system, IRAS observations in the 25 μm wave band showed that shape of the zodiacal cloud can be accounted for by a combination of about 1/4 to 1/3 asteroidal dust and about 3/4 to 2/3 cometary dust (Liou et al., 1995). In both cases, the particles are composed from different mixtures of solids. The emission features observed for several comets confirmed the presence of silicates, such as pyroxene and olivine (Swamy, 1986). The refractive index therefore changes from case to case and consequently it results in wide spread of the values of efficiency factors for scattering Q_{sca}, extinction Q_{ext} and radiation pressure Q_{pr}. These physical quantities, however, play a key role in dynamical evolution of dust particles and modify their lifetime in the solar system due to the P-R effect.

The corresponding radiation force consists of two terms. The first term $(1-\boldsymbol{v}\cdot\boldsymbol{e}_R/c)\ \boldsymbol{e}_R$ is generated by simultaneous action of the Doppler effect, the change of concentration of photons and the aberration of light, when the proper reference frame of the particle moves with velocity $\boldsymbol{v}$ with respect to the reference frame of the Sun; c is the speed of light and $\boldsymbol{e}_R$ is unit vector of the particle position with respect to the Sun. Simultaneous action of the Doppler effect and the change of concentration of photons corresponds to the change of flux density of radiative energy which can be found also from electromagnetic wave theory (Klačka, 1992). The second term in the P-R effect, i. e. P-R drag, comes from the aberration of light and its form is $-\boldsymbol{v}/c$, if the first order in v/c is used. The negative sign produces a kind of friction force and the particle slowly spirals toward the source of radiation.

However, the dust particles undergo also great temperature changes during they are moving around the Sun (especially at highly eccentric trajectories). The refractive index of some materials strongly depends on the grain temperature and thus it has an evident consequence on evolutional theory based on P-R effect. In spite of this fact, the temperature changes are still rarely assumed in numerical simulations. It is because of missing data on temperature dependency of dielectric function for astronomical materials. For instance, the extent to which the silicate dielectric function will depend upon temperature is also not well known (Draine and Lee, 1984).

At present, only a limited set of temperature dependent dielectric functions is available, e.g. for (amorphous) silicon or (amorphous) carbon. It is whenever a great motivation to evaluate temperature driven changes of optical properties also for this kind of (non)-astronomical materials of submicronic and micronic size, as the physics is the same for any material and thus our outcomes will be theoretically meaningful for further studies based on appropriate optical data. The paper focuses to optical properties of dust particles and their dependency on temperature at different heliocentric distances. Nevertheless, the main aim of the paper is *i*) to point out that orbital evolution of spherical particles composed of materials with temperature dependent refractive indices may differ from that evolution known as P-R effect, and *ii*) to give sufficient physical and numerical justifications for this claim.

2. Dielectric function

The optical functions of a material are often expressed in terms of the complex dielectric function ϵ or the complex refractive index m, where

$$m = \sqrt{\epsilon_1 + i\epsilon_2} = n + ik \quad . \tag{1}$$

Real and imaginary parts of the complex dielectric function $\epsilon = \epsilon_1 + i\,\epsilon_2$ are not independent, but they are constraint by Kramers-Kronig relation (Bohren and Huffman, 2004; Landau and Lifshitz, 1960). If for instance ϵ_2 is known, one can write Kramers-Kronig integral as follows

$$\epsilon_1(\lambda_0) = \frac{2}{\pi} P \int_0^{\infty} \frac{\lambda_0^2}{\lambda} \frac{\epsilon_2(\lambda)}{\lambda_0^2 - \lambda^2} \, d\lambda \quad , \tag{2}$$

where P indicates that the Cauchy principal value is to be taken. In general, the changes of dielectric function with temperature T may be due to temperature dependence of collision frequency ω_c or plasma frequency ω_p (Chiang et al., 1997). When relatively minor temperature dependence of density and effective mass of the electrons are neglected, the main variation of the dielectric function with T comes from temperature dependence of ω_c.

The optical constants for metallic particles can also depend on the size of granular structure. At least for small metallic grains, as shown by experiments with nanometer-sized silver spheres, it is known that the dielectric function can be influenced by grain size more efficiently than by the temperature (Kreibig, 1974). In contrary, the dielectric function of larger submicrometer- and micrometer-sized grains, typically present in interplanetary space, do not respond sensitively to changes of grain size or shape. Especially, the size-dependent effects in visual and near-IR being important for small clusters of some metals (e.g. silver as shown above) are negligible for pure iron possibly present in space (Kreibig and Vollmer, 1995). As for iron, the IR optical properties of larger grains with radii $R \gg 0.01 \mu m$ are affected by grain temperature (Fischera, 2004) due to the high Fermi velocity.

To determine the internal temperature of the grain, the basic assumption usually made is that all the factors tending to cause a change of temperature have reached equilibrium. Of the various processes leading to energy exchange between a grain and the surrounding medium, it was argued by (Wickramasinghe, 1967) that radiative process plays the dominant role in determining equilibrium grain temperature T_g. The temperature T_g can be obtained when solving an equation of the energy balance of the grain (Kocifaj et al., 2006). However, it has no sense to deal with temperatures greater than ≈ 1000 K, which can be reached close to the Sun, since particles evaporate in sufficiently intense radiation field (Mukai and Mukai, 1973). Namely, depending on dust composition, the evaporation of typical dust particles (except ices) occurs at temperatures 1000-2000 K (Wang and Wheeler, 1996; Ivezić et al., 1998).

3. Particle sources

Dust particles surviving for a long time in the interplanetary space are mainly released from comets and asteroids or are produced by fragmentation of larger cometary or asteroidal fragments (meteoroids). Emission features, observed in cometary dust in the IR have shown the presence of silicates, including crystalline olivine, and organics (Kolokolova and Jockers, 1997). However, comets are thought to be porous mixtures of dust and solidified water, carbon monoxide, carbon dioxide and hydrocarbons (Herique et al., 2002). Analysing the observational data, the presence of carbon and carbonaceous components in cometary material was deduced by various authors (Kolokolova et al., 2001; Moreno et al., 2003; Greenberg and Aigen, 1999). The contribution of other sources is small (Mann et al, 2004) so one can restrict the numerical modelling to the dust particles produced from comets, independent of whether they are released primary from comet or whether they are secondary collision products, produced in situ and then evolving dynamically, as described in this paper.

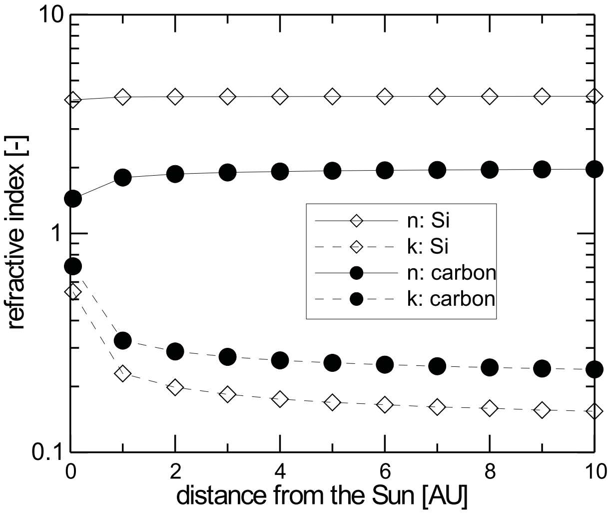

Figure 1. Refractive indices of amorphous silicon (at wavelength $\lambda = 0.6\ \mu m$) and amorphous carbon (at $\lambda = 0.5\ \mu m$) particles as a function of distance from the Sun.

Comets are usually expected to be a major source of dust inward from 1 AU. In particular, the role of several short period comets that approach relatively close to the Sun, i.e., P/Encke, is important because of their large contribution to the total mass input within 1AU (Ishimoto, 2000). From studies of stratospheric interplanetary dust particles it is clear that comet dust is not two independent populations of particles, one composed of pure C and the other of pure Si. Rather they are complicated amalgams, predominantly of silicate minerals, or oxidized minerals with SiO_3 or SiO_4. However, in the Introduction to the paper, Section 1, the motivation for studying silicon and carbon is accurately and acceptably presented: it is only considered because that is the only similar material for which the temperature variation of the dielectric function is known. This argument makes sense, and it justifies why the calculations are done with a material not considered astronomically significant.

The temperature dependent refractive indices for amorphous silicon (Do et al., 1992; Yavas et al., 1993) and amorphous carbon (Jäger et al., 2003) we used in numerical runs are drawn in Fig. 1 as a function of distance from the Sun. Although the real part of refractive index n for amorphous silicon varies only slightly with heliocentric distance, the imaginary part k undergos considerable change in the area with $r < 4$ AU (r is Sun-particle distance). The values of k for both, amorphous silicon and C particles, show the same decreasing trend with r, while n for C increases with r especially in the vicinity of the Sun.

4. Scattering and absorption of the light

Existence of the radiation pressure directly follows from Maxwell theory. The momentum removed from the incident electromagnetic radiation is proportional to C_{ext}, which relates to efficiency factor for extinction as follows $Q_{ext} = C_{ext}/(\pi R^2)$ (R is a particle radius). Part of removed energy is reradiated to the whole space 4π in form of scattered light ($C_{sca} = \pi R^2 Q_{sca}$). However, only forward scattered light is meaningful when evaluating the radial component of radiation pressure. Thus, one one hand it must be dealt with the contribution of forward projected momentum proportional to $\langle cos \rangle Q_{sca}$, where $\langle cos \rangle$ is so-called average asymmetry parameter. On the other hand, certain amount C_{abs} ($= \pi R^2 Q_{abs}$) is definitelly lost. In such a case, the pressure given on spherical particle by the flux of monochromatic radiative energy I_λ, is as follows

$$I_\lambda \pi R^2 (Q_{abs} + Q_{sca} - \langle cos \rangle Q_{sca}) \ , \tag{3}$$

where λ is the wavelength of incident radiation. The efficiency factors Q as well as the asymmetry parameter depend on λ, R and m in a complex way (Bohren and Huffman, 2004).

As shown in Fig. 2 for amorphous silicon and amorphous carbon, the spectral efficiency factor for extinction $Q_{ext}(\lambda = 0.55\ \mu m)$ depends on temperature variation only within the region $r < 1$ AU. Most important changes of Q_{ext} occur at $r < 0.5$ AU or for particles with sizes less than 1 μm. The reason of such behaviour is that Q_{ext} approaches quite fast its asymptotic profile when $x \equiv 2\pi R/\lambda \gtrsim 20 - 30$, i.e. at particle radii $R \gtrsim 2\ \mu m$. In spite of this fact, the Q_{ext} is not strictly a constant function of r for large particles, but has more-less a monotonous course in the inner regions of Earth's orbit. While Q_{ext} for amorphous silicon particles decreases with growing r, the Q_{ext} has increasing form for C particles. This fact indicates evident consequences on different evolutional aspects for amorphous silicon and amorphous carbon particles.

However, because of the polychromatic character of solar radiation, the total cross sections for scattering, absorption, extinction and radiation pressure of the particle are given by

$$\begin{aligned}
\bar{C}_{abs} &= \frac{\int_{\lambda_1}^{\lambda_2} I(\lambda)\ C_{abs}\ d\lambda}{\int_{\lambda_1}^{\lambda_2} I(\lambda)\ d\lambda} \ , \quad \bar{C}_{sca} = \frac{\int_{\lambda_1}^{\lambda_2} I(\lambda)\ C_{sca}\ d\lambda}{\int_{\lambda_1}^{\lambda_2} I(\lambda)\ d\lambda} \ , \\
\bar{C}_{ext} &= \frac{\int_{\lambda_1}^{\lambda_2} I(\lambda)\ C_{ext}\ d\lambda}{\int_{\lambda_1}^{\lambda_2} I(\lambda)\ d\lambda} \ , \quad \bar{C}_{pr} = \frac{\int_{\lambda_1}^{\lambda_2} I(\lambda)\ C_{pr}\ d\lambda}{\int_{\lambda_1}^{\lambda_2} I(\lambda)\ d\lambda} \ ,
\end{aligned} \tag{4}$$

where the interval $(\lambda_1,\ \lambda_2)$ covers the visible spectrum and the near infrared spectral band in this computational model. Although the 6000 K black-body model is realistic and very convenient as far as the numerical integration is concerned, it is inaccurate by as much as one order of magnitude in the region

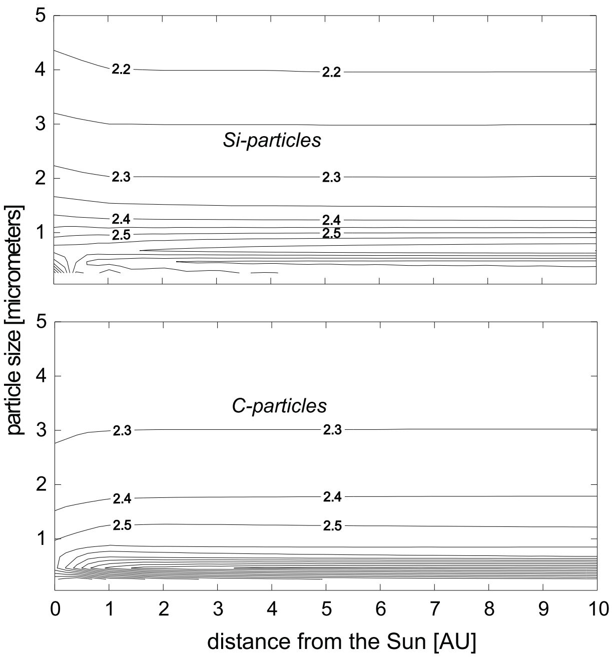

Figure 2. Efficiency factor for extinction for amorphous silicon and amorphous carbon spherules of different size calculated for monochromatic radiation with wavelength 0.55 μm.

$0.2 \leq \lambda \leq 0.6$ μm, a fact of considerable importance for the radiation pressure (Lamy, 1974). Therefore in this region $I(\lambda)$ was obtained from specific values given by (Neckel and Labs, 1981) and the rest curve in near-IR was substituted by an analytical function $A\lambda^{-\varrho} \exp\{-s\lambda^{-t}\}$, where coefficients A, ϱ, s, and t can be found in (Kastrov, 1979).

Integral values of efficiency factors needed for further computations then employ the form $\bar{Q}_{xxx} = \bar{C}_{xxx}/(\pi R^2)$, where xxx can be applied to scattering (sca), absorption (abs), extinction (ext) and radiation pressure (pr), respectively. Results of numerical runs for $\bar{Q}_{ext}$ and $\overline{\langle cos \rangle Q}_{sca}$ are presented in Figs. 3 and 4.

The structure of spectral and integral efficiency factors for extinction show some similar features:

- for amorphous silicon particles
  - Q_{ext} is a descending function of r close to the Sun
  - the most rapid changes are associated with the particles with size less than about 1 μm

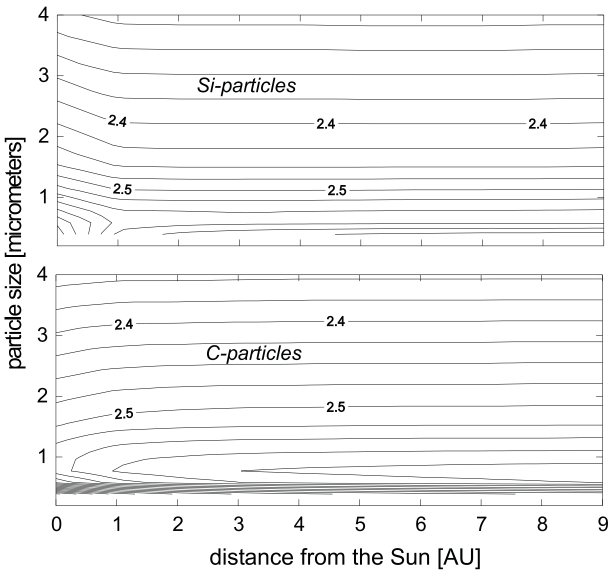

Figure 3. Integral values of efficiency factor for extinction in case of amorphous silicon and amorphous carbon particles having the spherical shape.

  - Q_{ext} is almost independent of heliocentric distance, when $r > 2$ AU
- for amorphous carbon particles
  - Q_{ext} is an ascending function of r close to the Sun
  - the particles less than about 1 μm in size are most significantly influenced by rapid changes of temperature close to the Sun
  - Q_{ext} is almost independent of distance from the Sun, when $r > 4$ AU and $R > 1.5$ μm

Whereas the optical response of the particle strongly depends on the size parameter $x = 2\pi R/\lambda$, the integration over the wavelengths (by means of Eqs. 4) results in a list of differences between spectral and integral values of efficiency factors for extinction (discussed above). The steep change of spectral functions Q_{ext} with R is evidently smoothed after integration over visible spectrum as seen from the structure of izolines in Figs. 2. and 3. For large particles ($R \gtrsim 1 - 2$ μm) the values of $\bar{Q}_{ext}$ are a bit larger than Q_{ext} for both types of materials. In accordance with very slight change of the product of Q_{sca} and $\langle cos \rangle$ with R (see Fig. 4), it inmplies increase of radiation pressure acting on these particles. Ascending form of $\bar{Q}_{ext}(r)$ for large amorphous carbon particles might swith over to descending form, when the particles occured less than 0.5 μm in size. This was not found for spectral values of Q_{ext}.

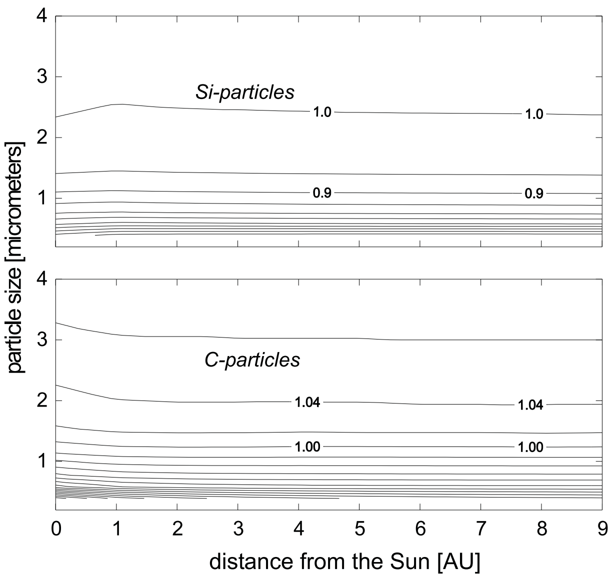

Figure 4. Integral value of the product of efficiency factor for scattering and asymmetry parameter in case of spherical particles composed of amorphous silicon and amorphous carbon.

The findings listed above have direct consequences on dynamical evolution of submicrometer- and micrometer-sized dust particles in the Solar System. The particles can account for greatest temperature-induced dynamical changes when they move at highly eccentric orbits. It is because of wide variation of distances from the Sun. Nevertheless, the particles will undergo most dramatic transitions at heliocentric distances less than 1 AU (as it is evident from Figs. 3 and 4). It is threfore of great interest to analyze just those dust populations which evolve at orbits with small perihelion distances.

5. Dynamical consequences of temperature dependent dielectric function

Radiation pressure force reduces the solar gravitational attraction acting on a particle (Robertson, 1937; Wyatt and Whipple, 1950; Harwit, 1963; Wilck and Mann, 1996; Jackson, 2001). Dominant part of acceleration of the particle is proportional to $-(1-\beta)\boldsymbol{r}/r^3$, where $\boldsymbol{r}$ is position vector of the particle with respect to the Sun, and β is a non-dimensional quantity often called the ratio of radiation pressure force to the gravitational force. The existence of velocity terms causes secular decrease of semimajor axis and eccentricity of the particle orbit (see also Mann et al, 2000). The evolution of the orbital motion cannot be analytically predicted when Q_{pr} varies with heliocentric distance r of the particle, and therefore it needs to be solved numerically.

Time evolution of spherical particles was simulated for amorphous silicon and amorphous carbon particles (as discussed in Sections 1 and 3), which started to evolve at orbits characterized by: semi-major axis a_P=2.2 AU, eccentricity e_P=0.85, inclination i_P=12.4°, longitude of the ascending node Ω_P=334.7°, and longitude of perihelion ω_P=186.3°. Since the micron-sized dust particles which "born" in close encounters with the Sun are immediately transferred to hyperbolic orbits (the perihelion escapes are well-known since the time of Harwit, 1963), the particles are assumed to be produced at large heliocentric distances ($r > 4$ AU).

We have made calculations for dust particles ejected with zero ejection velocities as the ejection velocities are negligible in comparison with the orbital velocity of the parent body (Hughes, 2000). In general, one can find that the influence of the ejection velocity (sunward and outward the Sun) usually does not play an important role for orbital evolution of micron-sized dust grains (Klačka et al., 2006). Considering zero ejection velocity, initial orbital elements of the particles are:

$$
\begin{aligned}
a_{in} &= a_P\,(1-\beta)\left(1 - 2\beta\frac{1 + e_P\cos f_P}{1\;-\;e_P^2}\right)^{-1} , \\
e_{in} &= \sqrt{1 - \frac{1 - e_P^2 - 2\beta\,(1 + e_P\cos f_P)}{(1-\beta)^2}} , \\
\cos(\Theta_P - \omega_{in}) &= \frac{\beta + e_P\cos f_P}{1-\beta}\;\frac{1}{e_{in}} , \\
\sin(\Theta_P - \omega_{in}) &= \frac{e_P\sin f_P}{1-\beta}\;\frac{1}{e_{in}} , \\
\Omega_{in} &= \Omega_P \;,\quad i_{in} = i_P \;,\quad \Theta_{in} = \Theta_P \;, \qquad (5)
\end{aligned}
$$

where $f_P \equiv \Theta_P - \omega_P$.

Runge-Kutta's method of the fourth order with the adaptive step-size was used for simulating the motion of amorphous silicon and amorphous carbon particles. It was shown that particles with sizes larger than 5 μm survive in the Solar System the same time independent of whether their dielectric functions depend on temperature, or whether they are strictly constant.

Real orbital evolution of spherical particle, under action of solar gravity and solar electromagnetic radiation is not very different from the approximation when radiation efficiency factors are considered to be temperature independent. As for evolution of semi-major axis and eccentricity, the differences in lifetimes are only several tenths of percent, for ≈ 2 μm dust grains. Of course, reality is different from approximation used up to now, if one deals with perihelion motion and inclination. While these orbital elements are characterized by constant values for the standard approach (i.e. di/dt=0 for inclination, and secular change of longitude of perihelion is $\langle d\omega/dt \rangle$=0), temperature dependent materials exhibit nonzero changes. We have found that changes of orbital elements are even more important if the effect of Lorentz force is taken into account. Inclination may differ in 5-20° from the case when optical properties are constant. Calculations for amorphous silicon and amorphous carbon particles yield changes of life-times up to several hundred years when particle size is about 2 μm. Importance of the effect of temperature grows for small particles when orbital evolution of submicron-sized grains is governed by simultaneous action of magnetic field and radiation force. This shows that simultaneous action of various effects (e.g., also other gravitational forces, mainly during close encounters with planets), can produce results which may be different from the case when temperature effects are ignored. Assuming a temperature dependence of the dielectric function it was found that the lifetime of small particles ($R < 1$ μm) is reduced by more than about 15% in comparison to particles with fixed optical constants. The difference between these lifetimes rapidly grows with decrease of particle radius (e.g. it is already 25% for $R = 0.8$ μm).

6. Conclusion

Interplanetary dust particles revolve the Sun in various heliocentric distances. These distances are characterized with different equilibrium temperatures of the dust grains. As the optical properties are functions of temperature, the properties are also function of the distance from the Sun. We have investigated efficiency factors for scattering and extinction (and also asymmetry parameter) for amorphous silicon and amorphous carbon particles as a function of heliocentric distance. The largest changes of these quantities occur in the zone close to the Sun, $r < 1.5$ AU, mainly for submicron meteoroids. While efficiency factor for extinction for C-particles is an increasing function of heliocentric distance in zone $r < 1.5$ AU, the same quantity for silicon-particles is a decreasing function. Opposite behaviour was found for the product of efficiency factor for scattering and asymmetry parameter. In future, it will be interesting to look at these quantities for more realistic materials and for more realistic shapes of the particles, mainly for nonspherical and porous/fluffy dust aggregates. Analogous investigations can be applied to dust envelopes around other stars, where also other wavelengths of electromagnetic spectrum may play an important role.

Application of the obtained optical results on dynamics of interplanetary micron-sized dust grains has shown the importance of temperature dependence mainly for high eccentric orbits with small perihelia and for simultaneous action of various gravitational and nongravitational effects.

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