On the Motion of Nonsymmetrical Particles with Nonuniform Active Surface in Rarefied Gas

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Abstract. The motion of solid particles in gas, rising because of nonuniform physicochemical processes on the surface of the particles is investigated. Using kinetic theory and solid body dynamic methods one can find that particle with convex nearly everywhere smooth surface, sorbing gas molecules nonuniformly over the surface (such as growing microcristalls) tends to move along the helix-like trajectory.

Keywords: solid particle, nonuniform active surface, rarefied gas, asymptotic trajectory.
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Most physicochemical processes (e.g. crystallization or heterogeneous chemical reactions) proceed nonuniformly by the solid-gas interface [1,2]. As had been shown by series of experiments, such nonuniformity can produce some force and torque having appreciable effect in solid particles dynamics.

In papers [3,4] the simplest model has been constructed for such a motion. There was considered the sphere-shaped particles, and model types of counteractions are specular reflection and sorption. Thereupon there was the general model of motion of solid body with nonuniform surface in gas was constructed, and the dynamical system for the bodies with arbitrary convex and smooth shape of surface was derived in papers [5,6]. Using these equations we shall investigated typical motion of solid particles in gas reacting nonuniformly over the surface. We suppose that another forces are negligible.

Let us consider rigid body of mass M , momentum P , inertia tensor $\hat{J}$, angular momentum K and center of mass R . Let us suppose that the shape of surface assigned by the equation $\varphi(r) = 0$ in center-of-mass system, which orts fixedly connected with rigid body and rotate with them, we shall denote these orts S_1, S_2, S_3 . Then we can use the following system [5]:

$$\begin{cases} \dfrac{dR}{dt} = V, \quad V = \dfrac{Q}{M}, \\ \dfrac{dS_j}{dt} = \left[\omega, S_j\right], \quad j = 1,2,3 \\ \dfrac{dQ}{dt} = \sum\limits_{i=e,d,s} \int \beta_i \cdot \Delta_i Q \cdot d\Omega, \\ \dfrac{dK}{dt} = \sum\limits_{i=e,d,s} \int \beta_i \cdot \Delta_i K \cdot d\Omega \end{cases}$$

Here the first and second equation are kinematic, they mean that the center of mass moves according current velocity and principal axes of inertia rotate according current angular velocity.

There are the force and torque in the right parts of next pair equations. Both of them are the fluxes of microscopic changes of momentum and angular momentum correspondingly. Properly the flux is resulted in summation over the all types of counteractions and integration over the all collisions on the surface with appropriate measure.

Let us consider this question in detail.

In fact the functions $\beta_i = \beta_i(r)$, $i = e, d, s$ depending upon point of surface are the weighting factors indicating relative contribution of each types of collisions: e - elastic or specular type, d - diffuse type, s - sorption. As being weighting factors the functions β_i must satisfy inequality $\beta_i \geq 0$ and form sum of unit: $\sum_{i=e,d,s} \beta_i \equiv 1$.

If we have molecule of mass m and momentum p colliding with surface, than the changes of momentum and angular momentum for various type collisions can be represented as follows [5]. The specular recoil gives:

$$\Delta_e Q = 2\left(M^{-1} + m^{-1} + \left([r,n], \hat{J}^{-1}[r,n]\right)\right)^{-1} \cdot (v,n)n$$
$$\Delta_e K = 2\left(M^{-1} + m^{-1} + \left([r,n], \hat{J}^{-1}[r,n]\right)\right)^{-1} \cdot (v,n)[r,n]$$

where n is inner normal in collision point. Averaging over reflected flux in case of diffuse scattering one can find:

$$\Delta_d Q = mv + n\sqrt{\tfrac{1}{2}\pi mkT_W}$$
$$\Delta_d K = m[r,v] + [r,n]\sqrt{\tfrac{1}{2}\pi mkT_W}$$

where T_W is the local temperature of surface. And the sorption gives:

$$\Delta_s Q = p$$
$$\Delta_s K = \frac{Mm}{M+m}[r, v + [\omega, r]]$$

The measure function or differential frequency $d\Omega$ can be defined as an average number of molecules in elementary phase volume $dr \cdot dp$ colliding with the outer boundary of body in unit time. It may be given by the following expression:

$$d\Omega = (v,n) \cdot \theta((v,n)) \cdot f(r,p)dp \cdot d\sigma, \quad d\sigma = |\nabla\varphi| \cdot \delta(\varphi(r)) \cdot dr .$$

Apparently this measure function depends upon geometry of solid body surface, local velocity of surface point, and distribution function $f(r,p)$. Here we shall consider Maxwellian distribution function with neglect of perturbation of solid body motion on the gas:

$$f(r,p) = f(p) = n_0 (2\pi mkT)^{-3/2} \cdot \exp\left(-\frac{p^2}{2mkT}\right)$$

Let us suppose that motion of solid particles is sufficiently slow in comparison with thermal velocity of gas molecules. This assumption is in agreement with the most of experimental conditions.

Now we can to integrate right parts of (1) over the momentum. Neglecting second order of smallness by Mach and Stroukhal numbers we find:

$$
\frac{dQ}{dt} = \mathrm{F}^{0} + \hat{D}V + \hat{C}\omega
$$
$$
\frac{dK}{dt} = \mathrm{M}^{0} + \hat{G}V + \hat{B}\omega
$$

Here the constant terms are:

$$
\begin{aligned}
\mathrm{F}^{0} &= \frac{n_0 kT}{2}\int\left(\frac{2\alpha}{m}\beta_e + \left(1+\sqrt{T_W/T}\right)\beta_d + \beta_s\right)\cdot n\cdot\sigma(r)dr \\
\mathrm{M}^{0} &= \frac{n_0 kT}{2}\int\left(\frac{2\alpha}{m}\beta_e + \left(1+\sqrt{T_W/T}\right)\beta_d + \frac{M}{M+m}\beta_s\right)\cdot[r,n]\cdot\sigma(r)dr
\end{aligned}
\qquad (3a)
$$

where $\alpha = \left(M^{-1} + m^{-1} + \left([r,n],\hat{J}^{-1}[r,n]\right)\right)^{-1}$;

The matrixes of coefficients in linear terms are:

$$
\begin{aligned}
\hat{D} &= -n_0\sqrt{\frac{mkT}{2\pi}}\int\left\{\kappa(r)\cdot n\otimes n^T + \beta_d\hat{I}\right\}\sigma(r)dr, \\
\hat{C} &= -n_0\sqrt{\frac{mkT}{2\pi}}\int\left\{\kappa(r)\cdot n\otimes[r,n]^T - \beta_d\hat{r}\right\}\sigma(r)dr, \\
\hat{G} &= -n_0\sqrt{\frac{mkT}{2\pi}}\int\left\{\left(\kappa(r) - \frac{m}{M+m}\beta_s\right)\cdot[r,n]\otimes n^T + \left(\beta_d + \frac{M}{M+m}\beta_s\right)\cdot\hat{r}\right\}\sigma(r)dr, \\
\hat{W} &= -n_0\sqrt{\frac{mkT}{2\pi}}\int\left\{\left(\kappa(r) - \frac{m}{M+m}\beta_s\right)\cdot[r,n]\otimes[r,n]^T + \beta_d\left(r^2\hat{I} - r\otimes r^T\right)\right\}\sigma(r)dr,
\end{aligned}
\qquad (3b)
$$

where $\kappa(r) = \frac{4\alpha}{m}\beta_e + \left(1+\frac{\pi}{2}\sqrt{T_W/T}\right)\cdot\beta_d + \beta_s$.

All matrixes (3b) are constant in frame of reference rigidly bound with solid body, therefore their elements depend upon a time in the fixed coordinate system because of solid body motion. This dependence can be described by following equations [5]:

$$
\frac{d\hat{X}}{dt} = \left\{\hat{\omega},\hat{X}\right\} = \hat{\omega}\hat{X} - \hat{X}\hat{\omega}, \qquad \hat{X} = \hat{J},\hat{C},\hat{D},\hat{G},\hat{W},
$$
$$
\frac{dY}{dt} = \hat{\omega}Y, \qquad Y = \mathrm{F}^{0},\mathrm{M}^{0}.
$$

One can get over this difficulty applying well known Euler change the frame of reference: centre point of new frame of reference coincides with center of mass and orts are directed along with principal axes of inertia. Such a change is linear transformation $Q = \hat{T}\widetilde{Q}$, $K = \hat{T}\widetilde{K}$, which matrix $\hat{T}$ is orthogonal and satisfying the following equation $\frac{d\hat{T}}{dt} = \hat{\omega}\hat{T}$. Its enables to find time dependence for all terms in the system (2,3):

$$\hat{X}(t)=\hat{T}(t)\hat{\tilde{X}}\hat{T}^{-1}(t), \qquad \hat{X}=\hat{J},\hat{C},\hat{D},\hat{G},\hat{W}$$
$$Y(t)=\hat{T}(t)\tilde{Y}, \qquad Y=\mathsf{F}^{0},\mathsf{M}^{0}$$

Let us apply this substitution of variables. Expressing forward and angular velocity via new variables (momentum and angular momentum with tilde respectively) one can finds:

$$\frac{d\tilde{Q}}{dt}=\tilde{\mathsf{F}}^{0}+M^{-1}\tilde{\hat{D}}Q+\tilde{\hat{C}}\tilde{\hat{J}}^{-1}\tilde{K}+[\tilde{Q},\tilde{\hat{J}}^{-1}\tilde{K}].$$
$$\frac{d\tilde{K}}{dt}=\tilde{\mathsf{M}}^{0}+M^{-1}\tilde{\hat{G}}Q+\tilde{\hat{W}}\tilde{\hat{J}}^{-1}\tilde{K}+[\tilde{K},\tilde{\hat{J}}^{-1}\tilde{K}]$$

So, now we have autonomous closed system of equations, there free terms and all matrixes are constant. The nonlinearity concealed in kinematic relations, now has developed obvious in gyroscopic terms.

Further supposing variables are given in rotating coordinates we shall leave out the tilde under the variables in order to avoid unhandiness:

$$\begin{cases}\dfrac{dQ}{dt}=\mathsf{F}^{0}+M^{-1}\hat{D}Q+\hat{C}\hat{J}^{-1}\tilde{K}+[Q,\hat{J}^{-1}K],\\ \dfrac{dK}{dt}=\mathsf{M}^{0}+M^{-1}\hat{G}Q+\hat{W}\hat{J}^{-1}K+[K,\hat{J}^{-1}K].\end{cases}$$

Let us consider some properties of system (4) and ascertain basic patterns of the solid body dynamics corresponding to the solutions of this system.

First, let us note, that absence of sorption (i.e. $\beta_s=0$) results in symmetry of matrixes of linear terms in right part of system (4) like Onsager principle manifestation: $\hat{G}=\hat{C}^{\mathsf{T}}$ (the matrixes $\hat{D}$ and $\hat{W}$ are symmetrical for any $\beta_i \;\; i=e,d,s$)

Second, let us consider kinetic energy $E=\dfrac{Q^2}{2M}+\dfrac{(K,\hat{J}^{-1}K)}{2}$ as a function of variables of the system (4) and its dependence upon a time. If we cast out free terms (later we shall reinstate it), then time derivative of kinetic energy in virtue of system (4) will be the quadratic form:

$$\frac{dE}{dt}=\left(V,\hat{D}V\right)+\left(V,\hat{C}\omega\right)+\left(\omega,\hat{G}V\right)+\left(\omega,\hat{W}\omega\right).$$

Here the substitution of matrixes (3b) gives the following expression:

$$\frac{dE}{dt}=-n_0\sqrt{\frac{mkT}{2\pi}}\int\left\{\kappa(r)\left(V+[\omega,r],n\right)^2+\beta_d\left(V+[\omega,r]\right)^2\right\}\sigma(r)dr+$$
$$+n_0\sqrt{\frac{mkT}{2\pi}}\cdot\frac{M}{M+m}\int\beta_s\left\{(\omega,r,V)-\frac{m}{M}(\omega,r,n)\left((\omega,r,n)+(V,n)\right)\right\}\sigma(r)dr$$

As is easy to see, if sorption factor β_s is sufficiently small (in accordance with usual experimental condition), than quadratic form (5) is negative definite. So, small-scale sorption results in energy decreasing in virtue of linear terms of the system (4), in turn quadratic (gyroscopic) terms have no action upon energy change (it is natural as their origin is the effect of frame of reference change).

Now, let us consider time derivative of kinetic energy in virtue of system wholly. In addition to quadratic form (5) linear terms is appear thereof free terms of system (4). How can they change time dependence of the kinetic energy? If absolute quantities of the system variables are small-scaled, then their influence is noticeable, and the special analysis is required to ascertain solution behavior. Else (if at least one component of variables is sufficiently large) then linear terms are the small correction regarding to quadratic terms and time derivative of kinetic energy be negative. So, exceeding some value kinetic energy decreases.

Hence one can deduce that small sorption factor results in uniformly boundedness of every solution then $t \longrightarrow \infty$, and boundedness of kinetic energy by some constant value depending upon the system coefficients (4).

Next, as right part of the system (4) defines smooth vector field in six-dimensional space $\{Q, K\}$, and every solution is uniformly bounded, the theorem on the transversal surface of vector field [7] is hold and there is at least one steady state solution of the system (4). This steady state solution is essential in the light of the next theorem.

Before the statement of this theorem some constants must be determined. Let the fist constant be $\vartheta = \inf\limits_{|V|^2+L^2|\omega|^2\neq 0} -\dfrac{(V,\hat{D}V)+(V,\hat{C}\omega)+(\omega,\hat{G}V)+(\omega,\hat{W}\omega)}{|V|^2+L^2|\omega|^2}$, where L - characteristic dimension of particle defined by the mass and maximal principal moment of inertia: $L = \sqrt{J_{\max}/M}$. And let us denote $\chi = \sqrt{J_{\max}/J_{\min}}$, where is the ratio of maximal principal moment of inertia to minimal principal moment of inertia in the square root.

Theorem [8]. If the square form (5) is negative defined and the next inequality holds:

$$\vartheta^2 > \tfrac{1}{\sqrt{2}}\chi M L^{-1} \cdot \sqrt{\mathsf{F}^{0\,2} + L^{-2}\mathsf{M}^{0\,2}}$$

Then there is the unique and globally stable solution of the system (4).

Let us explain the physical meaning of the statement of theorem: inequality appearing above holds in case of smallness of sorption factor or in case if sorption be sufficiently close to uniform. And the intense nonuniformity violates this inequality.

As a hypothesis one can surmise that this case our results remain qualitative valid. For the rigorous analysis higher order terms (by Mach and Stroukhal number) must be taken in to account, or alternative method of force and torque representation should be used.

So we have found a sufficient condition of global stability of the steady-state solution. The global stability means that any over solution tends to the steady-state solution then $t \longrightarrow \infty$. Thus we can find an asymptotic of coordinate trajectories of the solid body motion. Let (Q^∞, K^∞) be the steady-state solution of the system (4). In general case Q^∞ and K^∞ are the pair of two non-zero vectors. The corresponding velocities $V^\infty = M^{-1}Q^\infty$ and $\omega^\infty = \hat{J}^{-1}K^\infty$ are constant in rotating coordinates, therefore in the fixed coordinate system angular velocity ω^∞ is constant too, but forward velocity vector rotates over the angular velocity vector:

$$V(t) = \exp(\hat{\omega}^\infty t) \cdot V^\infty$$

Integrating over the time accurate with additive constant gives:

$$R(t) = V_{\parallel} t + \exp(\hat{\omega}^\infty t) \cdot R_{\perp}$$

where $V_{\parallel} = |\omega^\infty|^{-2}(V^\infty, \omega^\infty) \cdot \omega^\infty$, $R_{\perp} = |\omega^\infty|^{-2} \cdot [V^\infty, \omega^\infty]$. This is the motion by helical spiral with pitch $2\pi\,|V_{\parallel}|/|\,\omega^\infty\,|$ and radius $|R_{\perp}|$. In special cases helical spiral can degenerates to the straight line (if forward and angular velocities are collinear) or the circle (if velocities are perpendicular).

So, we found that if the sorption is small or nonuniformity of surface is feebly marked, then the trajectory of solid body with arbitrary convex surface moving in rarified gas and absorbing its molecules tends to be helix-like.

The constancy of the pitch and radius of helix is effect of our supposition of the constancy of surface properties and inertia characteristics (mass and inertia tensor) of solid body. In fact they are slowly changes and results in deformation of helixes. However, the qualitative behavior of motion is clear, also one should denote some experimental observations of helix-like trajectories presented in [9]. Earlier qualitative accordance of this experiment and simplest model has been discussed [3]. The simplest model gives helix-like trajectories too, but they are being intermediate asymptotics (not absolute asymptotics). Moreover the simplest model essentially implies the spherical shape of the body. In contrast to simplest model the result presented here in principle permits the quantitative comparison with the experiment as well as qualitative comparison. We hope that such experiments will appear in the future.

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REFERENCES

1. I. V. Melikhov, E. F. Simonov, A. A. Vedernikov, et al., *Khim. Fiz*. 41 (3), 5 (1997).
2. I. V. Melikhov, E. F. Simonov, and A. A. Vedernikov, *Zh. Fiz. Khim.* 72, 2300 (1998).
3. V. V. Vedenyapin, J. G. Batisheva,I. V. Melikhov, and A. Ya. Gorbatchevski, *Doklady Physics*, Vol. 48, No. 10, 2003, pp. 556–558.
4. J. G. Batisheva, V. V. Vedenyapin, I. V. Melikhov, and A. Ya. Gorbachevski, *Mat. Model.* 15 (6), 6 (2003).
5. Ya. G. Batisheva, *Doklady Physics*, Vol. 48, No. 10, 2003, pp. 587–589.
6. J. G. Batisheva. "On the motion of solid in gas reacting with its surface. Derivation of the dynamical system". Preprint of KIAM RAS, 2003, № 18, 23p.
7. B.A.Dubrovin, A.T.Fomenko, S.P.Novikov. "Modern Geometry. Methods and Applications". Springer-Verlag, GTM 104, Part 2, 1985.
8. J. G. Batisheva "The dynamics of solid in gas sorbing on its surface". Preprint of KIAM RAS, 2003, № 69, 25p.
9. Willneff J., Maas H.-G. // IAPRS, Vol. XXXIII, Amsterdam, 2000.