Kinetic equation including wave function collapses

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Abstract. A kinetic equation for probe particles colliding with buffer gas molecules is proposed, which is modified to include the concept of wave function collapse during particle collisions. Some consequences of such modification are discussed along with the possibilities for their observation.

1. Introduction

The nature of irreversibility continues to remain one of the most important fundamental problems of modern physics. The point of view that relates the irreversibility of evolution with the openness of physical systems seems to be the most satisfactory. A system subjected to observation is thereby principally open, i.e. it interacts with the surroundings possessing an unavoidable stochasticity. This makes a description of the system evolution by reversible equations only incomplete [1]. Thus it seems topical to construct a consistent theoretical description of the evolution of individual quantum objects interacting with the surroundings, which would include irreversible (jump-like or similar) changes of their vectors of state — wave function collapses.

Kadomtsev's hypothesis on self-modifications occurring at molecular collisions in gases [2], elaborated in detail in Refs [3, 4], has been an important step in obtaining quantitative estimates of the parameters of this process. According to this hypothesis, the wave function of a probe molecule after several successive collisions does not transform into a complex coherent superposition of scattered waves that exists in the total volume of the gas, but collapses into a well-localized (Gaussian) wave packet, which ultimately diffuses in the gas like a classical particle. The main result of these studies is a quantitative estimate of the stationary wave packet width, which appears to be of the order of

$$a = \sqrt{l\lambda_{th}} \,, \qquad (1)$$

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where l is the molecular mean free path, $\lambda_{th} = \hbar/(Mv_{th})$ is the thermal de Broglie wavelength, M is the molecular mass, and v_{th} is the characteristic thermal velocity.

In the present paper an attempt is made to estimate the effect of wave function collapses on the macroscopic properties of gas. To this purpose, we derive, based on the Kadomtsev hypothesis, an equation for the molecular density matrix in the Wigner representation. Papers [3, 4] provide the wave function equations modelling its collapse during the collision with a scattering centre of known position. Averaging over the positions of molecules whereupon a probe particle suffers collisions, requires a transit to a density matrix formalism. In such a formalism, we ignore the microstate of gas by stressing the essential details connected with the wave packet reduction.

2. Derivation of the kinetic equation

We wish to derive an equation for the density matrix of molecules representing a small admixture to the main gas component. For brevity we shall speak of probe particles in a buffer gas. The low concentration of probe particles means that we can neglect the interparticle interaction and consider their collisions with the buffer gas molecules only. Let $\hat{f}$ be the density matrix of a probe particle, $\hat{H}$ its Hamiltonian of free motion. After colliding with a buffer gas molecule, a probe particle turns out to be in a pure state $|\psi\rangle$, which in the coordinate representation takes the form

$$\langle \mathbf{r} | \psi \rangle = (\pi a^2)^{-3/4} \exp\left[-\frac{(\mathbf{r} - \mathbf{r}_0)^2}{2a^2}\right] \exp\frac{i\mathbf{p}_0\mathbf{r}}{\hbar} \,, \qquad (2)$$

where the Gaussian wave packet width a is given by Eqn (1). In the general case, the mean particle momentum $\mathbf{p}_0$ after a collision correlates with the mean $\mathbf{p}'$ before the collision. The point $\mathbf{r}_0$ at which the module of the function ψ reaches maximum is determined by the position of the scatterer and thus is a random quantity over which the averaging should be made.

The kinetic equation has the form

$$\frac{\partial \hat{f}}{\partial t} + \frac{i}{\hbar}(\hat{H}\hat{f} - \hat{f}\hat{H}) = -\hat{J}_{out} + \hat{J}_{in} \,, \qquad (3)$$

where $\hat{J}_{out}$ and $\hat{J}_{in}$ are the outcoming and incoming parts of the collision integral, respectively. First we consider $\hat{J}_{out}$.

The collision probability per unit time Γ of a probe particle with a buffer gas molecule is the ratio of the thermal velocity to the mean free path: $\Gamma = v_{th}/l$. Each collision, whether accompanied by a wave function reduction or not, brings the probe particle out of the initial state. Therefore,

$$\hat{J}_{out} = \Gamma \hat{f}. \tag{4}$$

Similarly, the incoming term may be written in a form following from the theory of jump-like random processes [5 – 7]:

$$\hat{J}_{in} = \Gamma \overline{\varkappa |\psi\rangle\langle\psi|}. \tag{5}$$

Here the overscribed bar indicates averaging over buffer gas states, i.e. over $\mathbf{r}_0$ and $\mathbf{p}_0$ entering Eqn (2). If a collision takes place with a certain buffer gas molecule, then the density matrix of the probe particle collapses to $|\psi\rangle\langle\psi|$. The probability of collision with this molecule is accounted for by the factor $\varkappa$. This dimensionless factor can be represented as a probability density for probe particles in a coordinate space integrated with a weight $|\psi|^2$:

$$\varkappa = V \int d\mathbf{r}' \, |\langle\mathbf{r}'|\psi\rangle|^2 \langle\mathbf{r}'|\hat{f}|\mathbf{r}'\rangle. \tag{6}$$

Here the total volume V of the system is introduced for normalization ($\varkappa$ is a dimensionless quantity). For further transformation of Eqn (6) we use Wigner representation (the arguments of the density matrix are the radius-vector and momentum) [8]. We assume that averaging over $\mathbf{p}_0$ and $\mathbf{r}_0$ can be done independently. Averaging over the scatterer coordinate amounts to integrating Eqn (6) over $\mathbf{r}_0$ and dividing by the total volume V, inside which molecules are distributed homogeneously. After substituting Eqn (1), $\hat{J}_{in}$ contains integral operators with kernels

$$K(\mathbf{p}, \mathbf{p}') = \left(\frac{a}{\sqrt{\pi}\,\hbar}\right)^3 \int d\mathbf{p}_0 \, \exp\left[-\frac{a^2(\mathbf{p} - \mathbf{p}_0)^2}{\hbar^2}\right] \Pi(\mathbf{p}_0|\mathbf{p}'), \tag{7}$$

$$\chi(\mathbf{r} - \mathbf{r}') = (2\pi a^2)^{-3/2} \exp\left[-\frac{(\mathbf{r} - \mathbf{r}')^2}{2a^2}\right]. \tag{8}$$

In expression (7), $\Pi(\mathbf{p}_0|\mathbf{p}')$ means a conditional probability density for the probe molecular state collapsing into a wave packet ψ with a given average momentum $\mathbf{p}_0$, provided that the probe particle momentum before the collision was equal to $\mathbf{p}'$.

The kernel $K(\mathbf{p}, \mathbf{p}')$ is the common probability of the probe particle changing momentum during the collision. Different forms of this kernel are discussed in the scientific literature (see, for example, Refs [9, 10]). We point here to its two main properties. Firstly, integrating it over $\mathbf{p}$ yields unity [which evidently follows from definition (7)]. Secondly, the form of the kernel is such that the probe particles kinetic equation containing it allows a stationary solution in the form of a Maxwellian distribution with the buffer gas temperature. In particular, in a strong collision model, $K(\mathbf{p}, \mathbf{p}')$ does not depend on $\mathbf{p}'$ at all and is defined as a normalized-to-unity Maxwellian distribution with the given temperature.

So, we can finally write down the kinetic equation which takes into account the wave function collapses during intermolecular collisions, as follows:

$$\frac{\partial}{\partial t} f(\mathbf{r}, \mathbf{p}, t) + \frac{\mathbf{p}}{M} \nabla f(\mathbf{r}, \mathbf{p}, t) = -\Gamma f(\mathbf{r}, \mathbf{p}, t)$$

$$+ \Gamma \int d\mathbf{r}' \int d\mathbf{p}' \, \chi(\mathbf{r} - \mathbf{r}') K(\mathbf{p}, \mathbf{p}') f(\mathbf{r}', \mathbf{p}', t). \tag{9}$$

This equation solely differs from the traditional one describing the evolution of a probe particle ensemble in a buffer gas [9, 10] in possessing an integral operator with kernel $\chi(\mathbf{r} - \mathbf{r}')$, which describes the nonlocality of the wave function collapse process during collisions. The traditional theory is local, which corresponds to a limiting transition $a \to 0$ and hence the degeneration of $\chi(\mathbf{r} - \mathbf{r}')$ into a δ-function (in this case the integration over the coordinate is trivial and does not occur in the final integro-differential equation for f). Note that the integration of χ over $\mathbf{r}$ yields unity. Due to these properties of both kernels K and χ, Eqn (9) conserves the matrix density normalization.

3. Some consequences

In the first place, consider the case when the hydrodynamic approximation is valid, i.e. inhomogeneities in the probe particles distribution have a space scale much greater than the mean free path. Since in a rarefied gas the thermal de Broglie wavelength is many orders of magnitude smaller than the mean free path, the w.f. collapse space parameter a turns out to be small with respect to the inhomogeneity space scale. This allows one to expand f under the incoming term integral in powers of $\mathbf{r} - \mathbf{r}'$. This is a conventional procedure for approximating an exact equation describing a discrete random process by a continuous random process governed by the Fokker – Planck equation [7].

Consider how the equation of continuity is modified. We introduce a density $\rho = M \int d\mathbf{p} f$ and a hydrodynamic velocity $\mathbf{u} = \rho^{-1} \int d\mathbf{p} \, \mathbf{p} f$. Then keeping terms to the second order inclusive we arrive at

$$\frac{\partial}{\partial t} \rho + \mathrm{div}(\rho\mathbf{u}) = D_c \Delta\rho. \tag{10}$$

Here Δ is the Laplace operator, and $D_c = 3\Gamma a^2/2$ is an anomalous diffusion coefficient due to the wave function collapses. In the equation of continuity

$$\frac{\partial}{\partial t} \rho + \mathrm{div}\,\mathbf{j} = 0,$$

the flux density should be written as

$$\mathbf{j} = \rho\mathbf{u} - D_c \nabla\rho.$$

The equations of energy and momentum transfer change in a similar way.

Let us estimate the contribution of new terms to hydrodynamic equations. Expressing Γ and a through the mean free path, we obtain the following remarkable result:

$$D_c = \frac{3\hbar}{2M}. \tag{11}$$

The anomalous diffusion coefficient turns out to be independent of the properties of the medium — temperature, probe matter and buffer gas densities — and is determined by the probe molecular mass M only. Estimating the latter as 10^{-22} g, we obtain $D_c \sim 10^{-5}$ cm^2 s^{-1}. This is much smaller than the

typical gas kinematic viscosity, which is of order $v_{\text{th}}l$. Thus, the presence of the wave function collapses does not practically change the results of hydrodynamic calculations on the evolution of macroscopic inhomogeneities in a gas, i.e. in this respect the hypothesis we used does not contradict experiment. At the same time, it serves as an irreversibility justification for such processes.

On the other hand, if an inhomogeneity oscillating with a period much less than a is formed in the probe particle spatial distribution, the corresponding integral in the right-hand side of Eqn (9) containing $\chi(\mathbf{r} - \mathbf{r}')$ vanishes, i.e. effectively only the outcoming term works, and during collapse such a homogeneity dissipates due to nonlocal effects very rapidly on a time scale of several Γ^{-1}. Such structures can be formed in the medium by an external electromagnetic field in resonance with some electronic transition in the probe molecule, if the field itself has a steady spatial structure (for example, as a monochromatic standing wave). Such structures are called laser-induced gratings [11, 12]. At room temperature $\lambda_{\text{th}} \sim 10^{-9}$ cm.

Suppose that the buffer gas is sufficiently rarefied and $l \approx 0.1$ cm. Then the collapse parameter $a \approx 10^{-5}$ cm and the laser-induced grating produced under ultraviolet radiation has a period s comparable with a. A nonlinear optical signal, obtained by diffracting the additional field on the laser-induced grating, carries information, in particular, on the difference of the Fourier transform of the kernel

$$\tilde{\chi} = \exp\left[-2\left(\frac{\pi a}{s}\right)^2\right]$$

from unity. However, the sensitivity of such a measurement is significantly limited by a number of both typically experimental and fundamental factors. For example, the finiteness of the laser beam radius causes a large time-of-flight broadening of the signal spectrum. On the other hand, if the grating formation and the signal wave generation are separated in time, the effect of the enhanced grating disruption we are interested in is smeared out by an inhomogeneous broadening of another type (the Doppler broadening). If the generation of the grating and signal occur continuously, then a source of irreversibility different from collisional one exists in the system, namely, spontaneous emission of photons (resonance fluorescence). This can significantly affect the type of molecular wave packet reduction. However, there is no principal prohibition to making an optical measurement capable of revealing the presence or absence of wave function collapses during collisions. But the precision of experimental methods inherent in nonlinear laser spectroscopy must be significantly improved in order to achieve this goal (preliminary estimates show that the necessary accuracy of the signal power measurements should be below the 1% level).

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