PFC/RR-86-24

DOE/ET-51013-204
UC20,f

Techniques for Obtaining Velocity Distributions of Atoms or Ions from Doppler-broadened Spectral Line Profiles

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December 1986

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Abstract

Analysis of the doppler-broadened profiles of spectral lines radiated by atoms or ions in plasmas yields information about their velocity distributions. Researchers have analysed profiles of lines radiated by atoms in isotropic velocity distributions in several ways, one being the inversion of the integral equation which relates the velocity distribution to the line profile. This inversion formula was derived for a separate application and was given to within an arbitrary multiplicative constant. This paper presents a new derivation which obtains the inversion exactly, using a method which is easily generalized for determination of anisotropic velocity distribution functions. The technique to obtain an anisotropic velocity distribution function from line profiles measured at different angles is outlined.

I. Introduction

High resolution spectroscopy of lines radiated by atoms or ions in plasmas reveals information about their velocity, or energy, distributions. Researchers have obtained highly resolved spectra of line radiation to determine the presence of atoms arising from molecular dissociation or charge exchange in plasma discharges. McNeil et.al. [1-3] have measured the Hα line profile under high resolution in the PDX tokamak and in ion source discharges and noted the departure of those profiles from those which would result from a thermal velocity distribution. They proposed distributions consisting of linear combinations of isotropic thermal and non-thermal component distributions functions and fit the coefficients multiplying these functions to match the measured spectrum. Freund, Shiavone and Brader[4] measured the Hα, Hβ, Hλ, and Hδ line profiles of excited atoms dissociated from H_2 by an electron beam. These line shapes had a central "cold" peak on top of a broad, flat profile radiated by the "hot" component. The relative areas under these two profiles were compared to give the proportion of "hot" to "cold" atoms. Higo, Ogawa and Kamata[5] and Higo and Ogawa[6-8] measured the line profiles of Hα and Hβ from excited atoms produced by controlled electron impact on H_2 and HCL. They assumed the atoms were in an isotropic velocity distribution and applied the formula derived by Durop and Heitz[9] to obtain the relative energy distribution of the emitting atoms.

This formula was derived as a special case of the general problem of measuring the isotropic velocity distribution of ions coming from a volume of dissociating atoms and having velocities directed into a given solid angle. The experiment measured $f(v')dv'$, the probability of finding a particle with velocity between v' and $v'+dv'$ within the solid angle of collection. When the area of collection becomes an infinite plane, the problem is identical to the one of inferring the velocity distribution of atoms or ions from a measurement of the doppler-broadened line profile.

Since the mathematical apparatus used in deriving this inversion was developed for use in solving a more general problem, the treatment is more complicated than is needed to solve the problem addressed here, and furthermore, it leaves an undetermined multiplicative constant. This paper presents a more staightforward derivation of the inversion which obtains it exactly. The inversion is demonstrated on a sample distribution.

When the velocity distribution is not isotropic the above mentioned inversion cannot be used. In that case, one may obtain enough information to determine the velocity distribution by viewing the emitting volume from several angles and measuring the profiles of spectral lines radiated by the atoms or ions. This data could then be used to obtain the three dimensional velocity distribution using a technique the author calls "doppler-shift velocity-space tomography". This method is outlined in section III.

II. Derivation

A photon radiated by an non-relativistic atom moving with velocity v and radiating into a direction which makes an angle θ with respect to its velocity will be doppler-shifted by an amount $\Delta\lambda = \lambda\ v/c \cos\theta$ where λ is the wavelength radiated by the atom at rest and c is the speed of light. If photons are observed from only one direction, z, and v_z is the component of velocity in that direction, then $\Delta\lambda = \lambda\, v_z/c$. Then, if $f(v_z)dv_z$ is the number of radiating atoms in the emitting volume with z-components of velocity between v_z and $v_z + dv_z$,

$$f(v_z)dv_z = H(\Delta\lambda)d(\Delta\lambda) \tag{1}$$

where $H(\Delta\lambda)d(\Delta\lambda)$ is the number of radiated photons with wavelength shifts between $\Delta\lambda$ and $\Delta\lambda + d(\Delta\lambda)$. Since $\Delta\lambda=\lambda\, v_z/c$, $d(\Delta\lambda) = \lambda/c\; dv_z$ and

$$f(v_z) = H(\Delta\lambda)\; \lambda/c \tag{2}$$

So, a measurement of $H(\Delta\lambda)$ gives $f(v_z)$. $f(v_z)$ is related to the three dimensional velocity distribution function $F(v_x,v_y,v_z)$ by the equation

$$f(v_z) = \int\!\!\int F(v_x,v_y,v_z)dv_x dv_y \tag{3}$$

where $F(v_x,v_y,v_z)dv_x dv_y dv_z$ is the number of particles with velocities between v_x and $v_x + dv_x$, v_y and $v_y + dv_y$, and v_z and $v_z + dv_z$, and the integration is over all v_x and v_y for which $F(v_x,v_y,v_z) > 0$. If the distribution is isotropic in velocity space, then $F(v_x,v_y,v_z) = F(v)$ where $v^2 = v_x^2 + v_y^2 + v_z^2$. The distribution is then spherically symmetric in velocity space with a probability density which depends only on the magnitude v, and which has a maximum radius v_m corresponding to the maximum $\Delta\lambda$ for which $H(\Delta\lambda)$ is non-zero, $\Delta\lambda_m$.

$$v_m = \Delta\lambda_m c/\lambda \tag{4}$$

(See figure 1). The integral $f(v_z')$ for a particular v_z' extends over the "disk" marked a, which is centered at $(0,0,v_z')$ and is in a plane parallel to the v_x,v_y plane. For each v_z then, $f(v_z)$ is the integral of F(v) over a "slice" through the velocity space sphere . Thus, a measurement of $f(v_z)$ at n different v_z's is equivalent to measuring the integral of F(v) over n "slices", each in a plane parallel to the v_x,v_y plane. This is analogous to measuring the integral of the electron density or spectral brightness over a slab in a spherically symmetric "real space" plasma and inferring the radial distribution of these quantities from measurements made over many slabs, ie., the three dimensional equivalent of the Abel inversion. This analysis can be generalized to the case where the distribution function is not Bpherically symmetric as will be shown in section III.

For the case of a spherically symmetric distribution function, the inversion formula relating F(v) to $f(v_z)$ can be simply obtained. Let $v_\perp^2 = v_x^2 + v_y^2$. Then, from equation (3)

$$f(v_z) = \int_0^{(v_m^2 - v_z^2)^{1/2}} F(v) 2\pi v_\perp dv_\perp \ . \tag{5}$$

Since $v^2 = v_\perp^2 + v_z^2$, $vdv = v_\perp dv_\perp$ for fixed v_z. Then,

$$f(v_z) = 2\pi \int_{v_z}^{v_m} F(v)vdv \tag{6}$$

Now define a function g(v) where g(v)dv equals the number of particles with speeds between v and v + dv. Then

$$g(v)dv = 4\pi v^2 F(v)dv \tag{7}$$

and

$$F(v) = \frac{g(v)}{4\pi v^2} \tag{8}$$

So that

$$f(v_z) = 1/2 \int_{v_z}^{v_m} \frac{g(v)}{v} dv \tag{9}$$

Inspection of this equation shows that $f(v_z)$ will be a monotonically decreasing function for any g(v).

If g(v) represented a monoenergetic particle distribution, ie. $g(v) = A\delta(v-v_o)$, then

$$f(v_z) = \frac{A}{2v_o} \qquad \text{if} \quad v_z < v_o \tag{10}$$

and $$f(v_z) = 0 \qquad \text{if} \quad v_z > v_o$$

The measured line profile $H(\Delta\lambda)$ will then be a step function, constant for $-v_o\lambda /c < \Delta\lambda < v_o\lambda /c$ and zero elsewhere.

Differentiating both sides of equation (9) and evaluating at $v_z = v$ gives

$$\frac{df(v)}{dv} = -1/2\, \frac{g(v)}{v} \tag{11}$$

So that

$$g(v) = -2v\, \frac{df(v)}{dv} \ . \tag{12}$$

Applying this inversion on the step function, equation (10), then gives $g(v) = A\delta(v-v_o)$, the monoenergetic distribution function.

In terms of $H(\Delta\lambda)$,

$$g(v) = \frac{-2\lambda\Delta\lambda}{c}\, \frac{dH(\Delta\lambda)}{d(\Delta\lambda)} \ . \tag{13}$$

The kinetic energy distribution G(E) where G(E)dE is the number of radiating particles with energies between E and E + dE is given by

$$G(E)dE = g(v)dv \ . \tag{14}$$

Therefore,

$$G(E) = \frac{-2\lambda^2}{mc^2}\, \frac{dH(\Delta\lambda)}{d(\Delta\lambda)} \tag{15}$$

where m is the mass of the radiating particle.

So, a measurement of $H(\Delta\lambda)$ can be differentiated to obtain G(E), the kinetic energy distribution.

As mentioned, the above derived inversion technique applies only to line profiles which are radiated by particles in an isotropic velocity distribution and for which the broadening is due only to doppler shifts. The line may be broadened by Zeeman splitting, Stark broadening, fine structure, or finite instrumental resolution. Higo and Ogawa presented the results of a relative measurement of G(E) vs. E, inferred from a measurement of the Hα line profile [6-8] made under conditions in which the line broadening was almost all kinetic in origin, and using the inversion derived in ref.9, which is the same as eq.15 except for the multiplicative constant. The data were presented with an energy resolution of approximately .15 ev, which is the best resolution which could be obtained in this case, owing to the fine structure splitting of the Hα spectral line.

III. Inversion of Anisotropic Distributions

A hydrogen atom in a plasma can charge-exchange with a plasma proton. In that case, the new atom will have the velocity of the original ion. This process can create a population of highly energetic atoms which has the characteristics of the ion velocity distribution. If the ion velocity distribution is anisotropic, such as the loss-cone distribution in a magnetic mirror or a toroidally drifting distribution in a tokamak, the highly energetic component of the neutral velocity distribution will be anisotropic as well. The doppler-shifted light radiated by these atoms will show these anisotropies. Light from toroidally drifting hyrdrogen atoms has been observed in tokamaks and used to determine drift velocity.[10]

If the radiating atoms or ions are not isotropic in velocity space, then the above derived inversion does not apply. In that case more than one view is needed to determine $F(v_x, v_y, v_z)$. As in the case of the isotropic inversion, a view along the z axis gives $f(v_z)$ where

$$f(v_z) = \iint F(v_x, v_y, v_z)\, dv_x dv_y \tag{16}$$

and f is defined as in section II and the area of integration is the same as in equation (3). Again, dividing the v_z axis into increments, $f(v_{zi})$ is the integral of $F(v_x, v_y, v_z)$ over the i'th slice centered at $(0, 0, v_{z_i})$ and parallel to the v_x, v_y plane. If $f(v_z)$ is known at n different v_z' s, then the integral of $F(v_x, v_y, v_z)$ is known over n "slices" through the velocity distribution, which can be thought of as an "object" of varying density in a three dimensional velocity space. An example is shown in figure 2a. This is analogous to spatial tomography in which measurements of emission or absorption are made along chords through a plasma[11] or a human body[12] and from which the emission or absorption function is inferred.

The line profile can be measured along the x axis to yield $f'(v_x)$ where

$$f'(v_x) = \iint F(v_x, v_y, v_z)\, dv_y dv_z \tag{17}$$

For each v_{x_1}, $f'(v_{x_1})$ is the integeral of $F(v_x, v_y, v_z)$ over the "slice"centered at $(0, 0, v_{x_1})$ and parallel to the v_z, v_y plane. (See figure

2b). This could be done also for v_y or any arbitrary velocity direction $\hat{v}$. Each measured line shape yields a set of equations. For example, a measurement of $H(\Delta\lambda)$ at n different $\Delta\lambda$'s yields n equations.

$$f(v_{z_1}) = \iint F(v_x, v_y, v_{z_1})\, dv_x dv_y \tag{18}$$

$$f(v_{z_2}) = \iint F(v_x, v_y, v_{z_2})\, dv_x dv_y$$

$$\cdot \qquad\qquad \cdot$$

$$\cdot \qquad\qquad \cdot$$

$$f(v_{z_n}) = \iint F(v_x, v_y, v_{z_n})\, dv_x dv_y$$

where $f(v_{z_1}) \propto H(\Delta\lambda_1)$ and $\lambda_1 = \lambda\, v_{z_1}/c$. Likewise, measurments of the line profile along different directions yield similar sets of equations. As in "real space" tomography, these equations can be solved by proposing a form for F which is a linear combination of the functions P_k.

$$F(v_x, v_y, v_z) = \sum_{k=0}^{k_{max}} B_k\, P_k(v_x, v_y, v_z) \tag{19}$$

Each integral for $f(v_{z_1})$, for example, yields

$$f(v_{z_1}) = \sum_{k=0}^{k_{max}} C_{k, v_{z_1}} B_k \tag{20}$$

where

$$C_{k,v_{z_1}} = \iint P_k(v_x,v_y,v_z)\ dv_x dv_y \tag{21}$$

and the integration is over the area in the v_x, v_y plane for which F is > 0. This area is determined by measuring the line profile in the x and y directions and obtaining the maximum v_x and v_y of the distribution which correspond to the maximum $\Delta\lambda$ of the line profile measured along the x and y directions respectively. If the number of equations of type (20) is greater than k_{max}, then the coefficients B_k may be determined by least squares analysis. The form of the functions P_k chosen will depend upon the number and angular distribution of the available views through the plasma. More angular information about the distribtuion function will require more views at different angles. Because of its similarity to real-space tomography, this technique may be called "doppler-shift velocity-space tomography". This differs from real-space tomography in that with real-space tomography the absorption or emission function of the real-space object is inferred from measurents of the average emission or absorption along chords through the "object", while with "doppler-shift velocity-space tomography" the density of the velocity-space "object" is inferred from measurments of the average density over planes which slice through the velocity-space "object".

IV. Summary

The velocity, or energy, distributions of radiating atoms or ions which are moving isotropically may be obtained by measuring the doppler-broadened line emission wavelength profile and applying the mathematical inversion derived here as long as the line broadening is essentialy kinetic in origin.

The velocity distributions of radiating atoms or ions which are not moving isotropically, and for which the broadening is kinetic in origin, may be obtained by viewing the emitting plasma from multiple angles and employing the "doppler-shift velocity-space tomography" technique outlined here. Experiments to investigate the velocity-space distributions of radiating hydrogen atoms in the Tara Tandem Mirror plasma confinement experiment using these techniques have begun.

References

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Figure Captions

Figure 1. A spherical velocity-space distribution. The shaded disk a is the area over which the integration of F(v) is carried out to obtain f(v').

Figure 2a. Anisotropic velocity distribution showing the "slices" through the distribution function over which $F(v_x,v_y,v_z)$ is integrated to obtain $f(v_z)$.

Figure 2b. Anisotropic velocity distribution showing the "slices" through the distribution function over which $F(v_x,v_y,v_z)$ is integrated to obtain $f'(v_x)$.

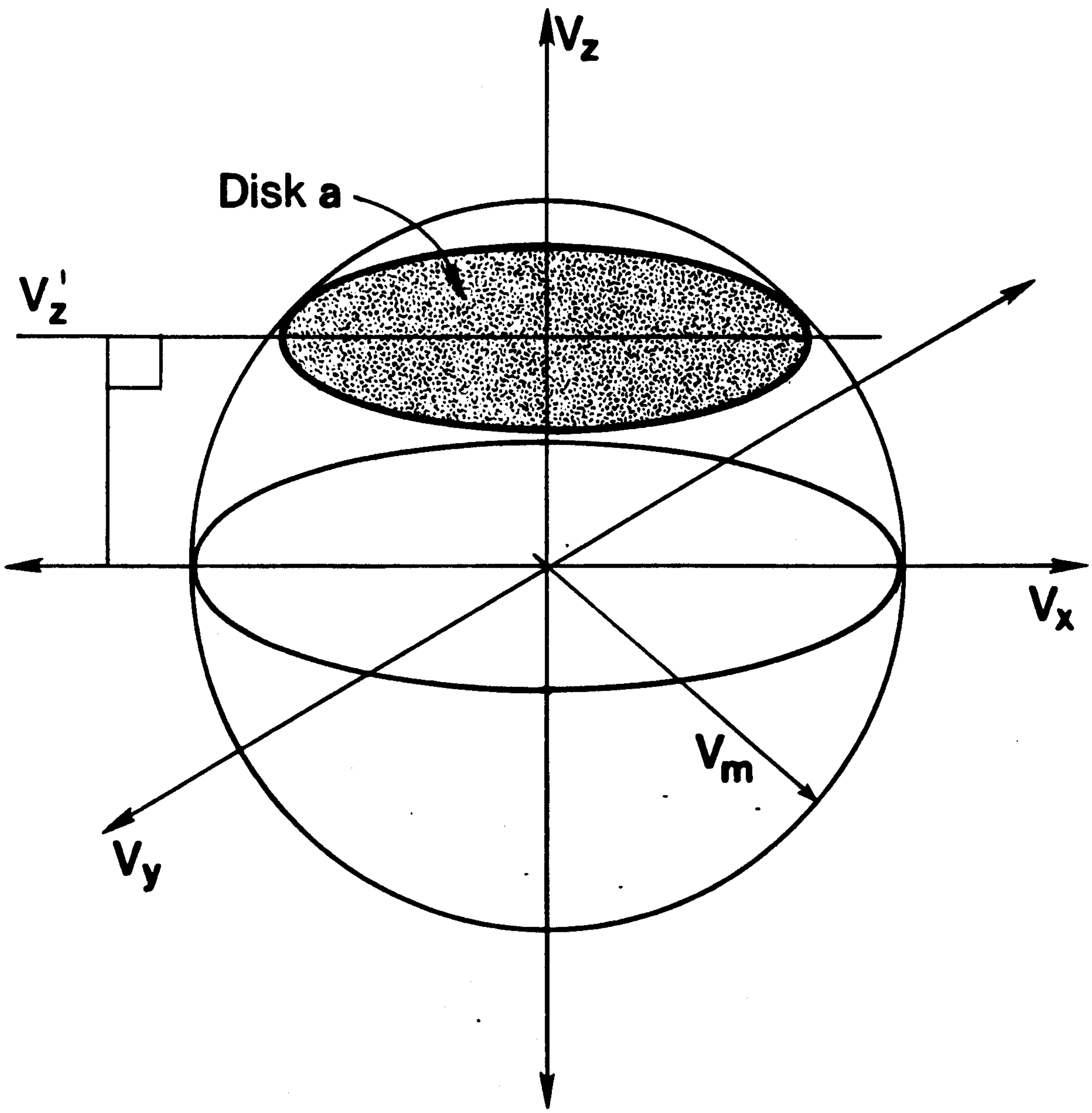

Fig. 1

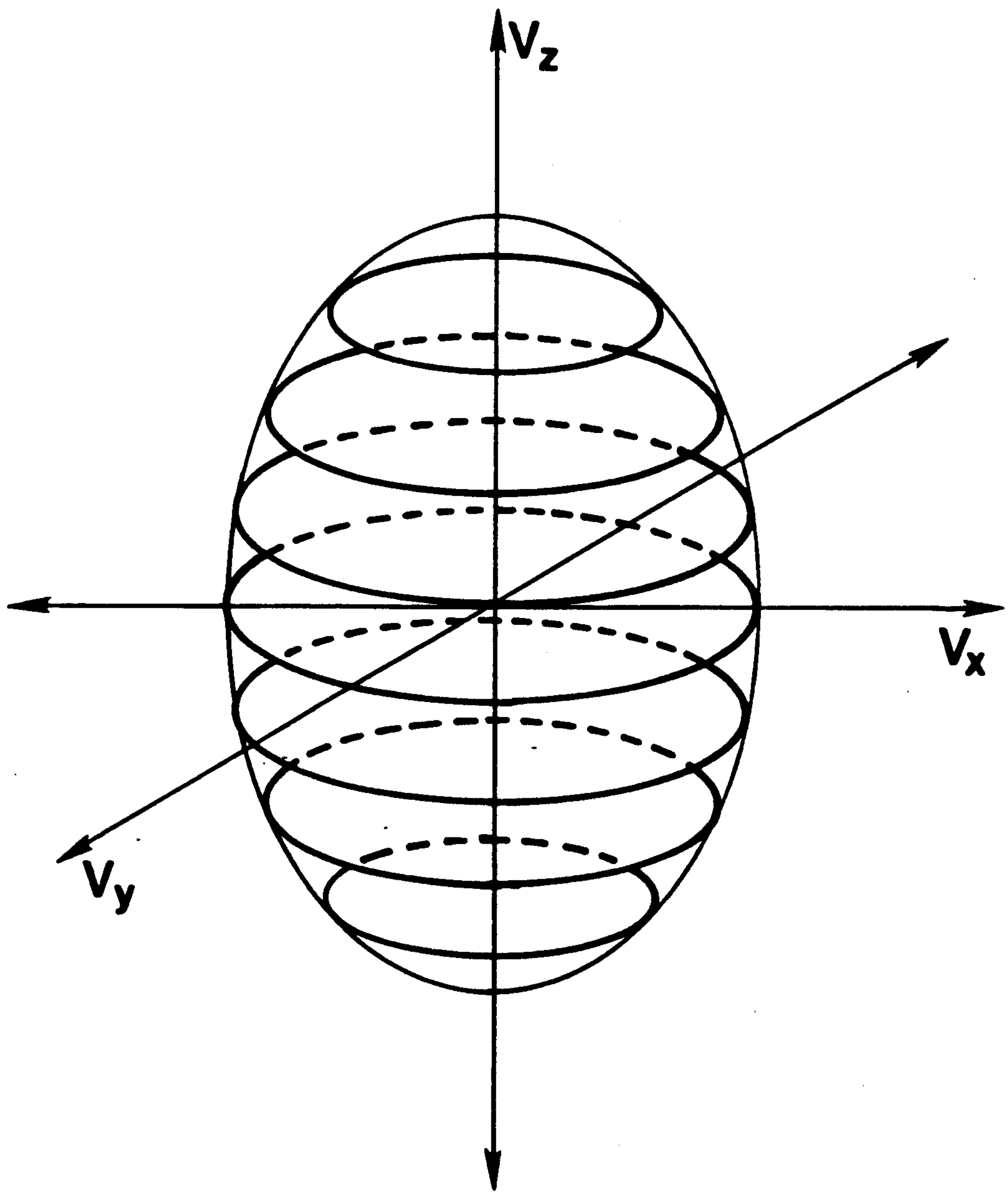

Fig. 2a

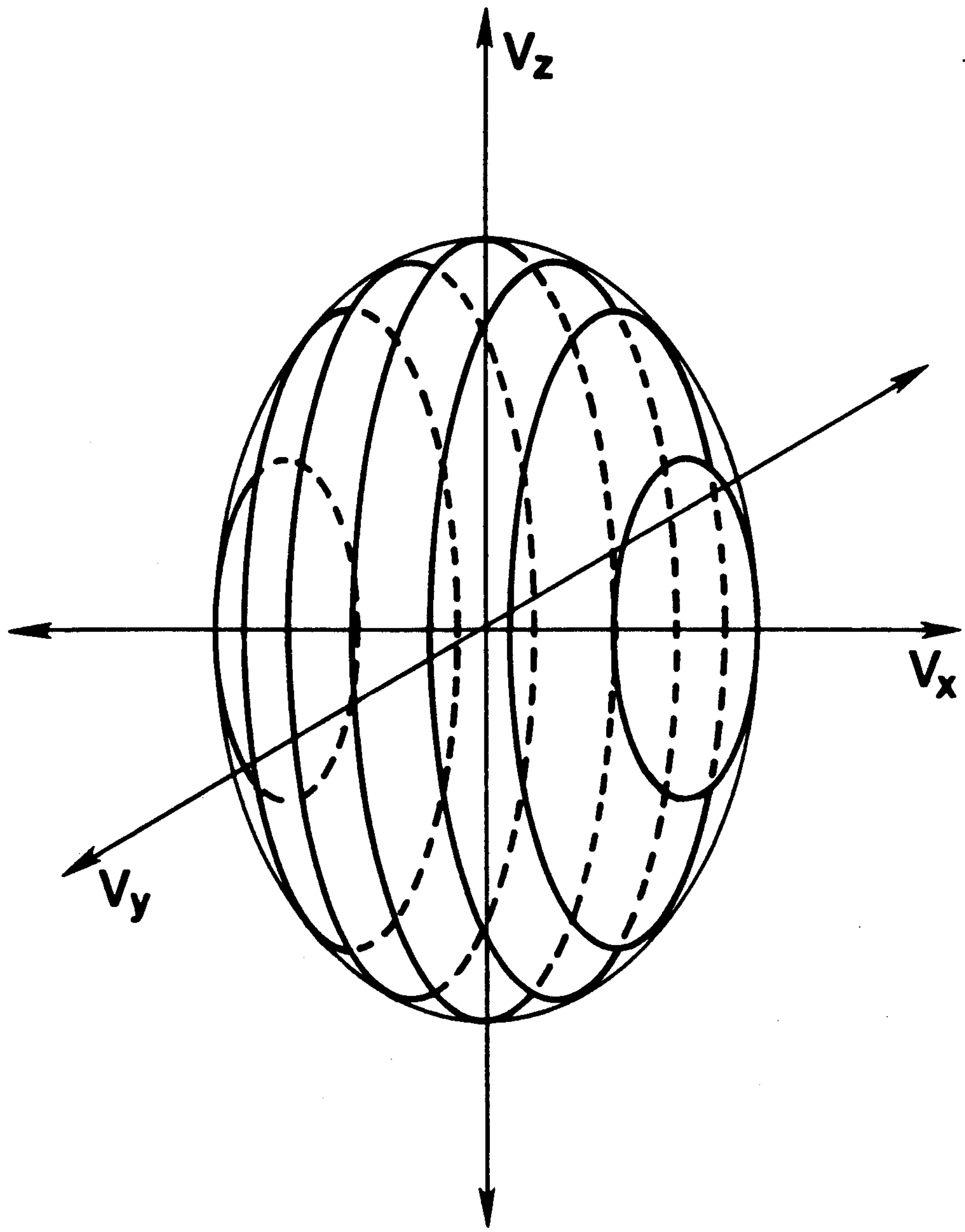

Fig. 2b