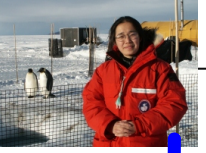
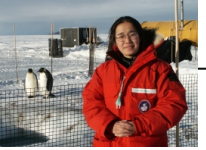


Lecture 12. Temperature Lidar (1) Overview and Physical Principles

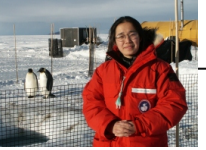
- Concept of Temperature
  - Maxwellian velocity distribution & kinetic energy
- Temperature Measurement Techniques
  - Direct measurements: velocity distribution & average
  - Temperature-dependent & sensitive effects
- Temperature Measurements with Atmospheric Lidars
  - Doppler Technique
  - Boltzmann Technique
  - Integration Technique
- Summary



Concept of Temperature

Temperature is a measure of the statistical average kinetic energy of particles (atoms or molecules) under thermodynamic equilibrium.

- Thermodynamics – The thermodynamic temperature is a state variable that describes the degree or intensity of thermal motions or internal heat presented in a substance or object. The temperature of two systems is the same when the systems are in thermal equilibrium.
- Collisions are the key in establishing the state of thermal equilibrium and determining molecule velocity distribution, especially for gas phase substance. Because of collisions, energy is equally partitioned among different degrees of freedom in classical physical picture.
- In classical statistical physics where energy is continuous– each independent degree of freedom possesses the same average kinetic energy $k_BT/2$, which is called the theorem of equipartition of energy. The individual molecule's kinetic energy or velocity may be quite different from the statistical average at any instantaneous time, but an average over a large amount of molecules leads to the same kinetic energy in different degrees of freedom, like translational, rotational and vibrational motions.



Concept of Temperature

The absolute (thermodynamic) temperature is a measure of the statistical average kinetic energy in each independent degree of freedom for atoms or molecules under thermodynamic equilibrium.

- In classical statistical physics,

1) A mass point has three degrees of freedom in translational motion:

translational kinetic energy $\frac{1}{2}m\overline{v^2} = \frac{3}{2}k_B T$

2) A rigid body has extra three degrees of freedom in rotational motion:

translational kinetic energy $\frac{1}{2}m\overline{v_x^2} = \frac{1}{2}k_B T$ for one DOF

rotational kinetic energy $\frac{1}{2}I\omega^2 = \frac{1}{2}k_B T$ for one DOF

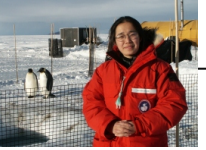
3) Molecules (diatomic) with rotational and vibrational motions:

translational kinetic energy $\frac{3}{2}k_B T$

rotational kinetic energy $k_B T$

vibrational kinetic energy $\frac{1}{2}k_B T$

vibrational potential energy $\frac{1}{2}k_B T$



Maxwellian Velocity Distribution

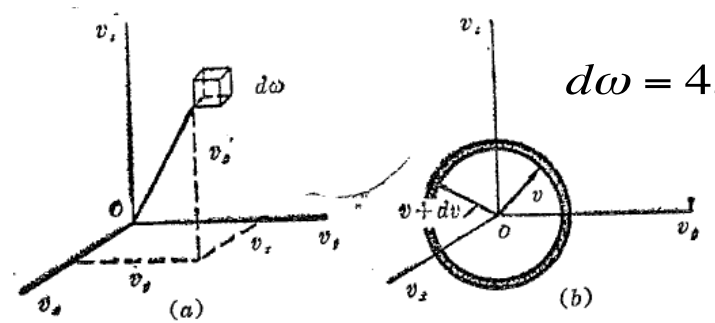
The Maxwellian velocity distribution of molecules is a statistical law under thermodynamic equilibrium established by collisions among molecules.

- Maxwellian velocity distribution:

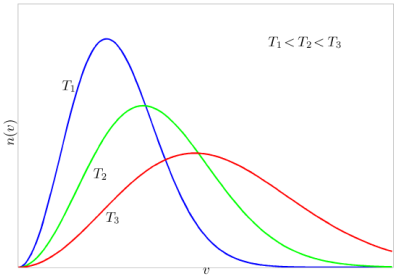
$$f(v_x) = \frac{dN(v_x)}{N dv_x} = \left(\frac{m}{2\pi k_B T}\right)^{1/2} e^{-mv_x^2/2k_B T}$$

$$f(v_y) = \left(\frac{m}{2\pi k_B T}\right)^{1/2} e^{-mv_y^2/2k_B T}$$

$$f(v_z) = \left(\frac{m}{2\pi k_B T}\right)^{1/2} e^{-mv_z^2/2k_B T}$$



$$d\omega = 4\pi v^2 dv$$



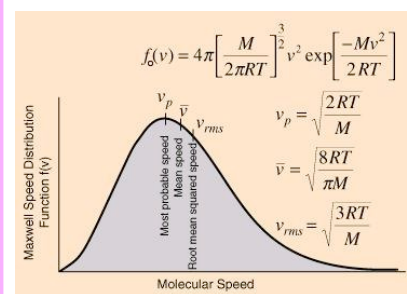
- Maxwellian speed distribution:

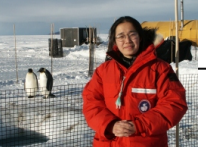
$$f(v) = 4\pi \left(\frac{m}{2\pi k_B T}\right)^{3/2} e^{-mv^2/2k_B T} v^2$$

$$\sqrt{\overline{v^2}} = \sqrt{\int_0^\infty v^2 f(v)\,dv} = \sqrt{\frac{3k_B T}{m}}$$

$$\bar{v} = \int_0^\infty v f(v)\,dv = \sqrt{\frac{8k_B T}{\pi m}}$$

$$v_p = \sqrt{\frac{2k_B T}{m}} \quad for \quad \frac{df(v)}{dv} = 0$$

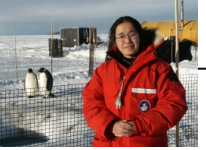




Concept of Temperature

Temperature is a measure of the statistical average kinetic energy of atoms or molecules under thermodynamic equilibrium, but the equipartition theorem breaks down in quantum world because many energy levels are no longer continuous but discrete and when the thermal energy k_BT is significantly smaller than the spacing between energy levels.

- In solids where there is no translational or rotational motion, temperature is a measure of the average vibrational kinetic energy.
- In ideal gas where there are no interactions among molecules except collisions that are elastic, temperature is mainly a measure of translational kinetic energy because collisions concerning translational motions are essential to establish thermodynamic equilibrium. However, as long as the energy level spacing is smaller than the thermal energy k_BT, the classical equipartition of energy is still valid (approximately) so then other degrees of freedom share the similar kinetic energy, the similar temperature.
- Temperature concept can be defined to tailor specific motion's kinetic energy, e.g., vibrational temperature or spin temperature, etc.



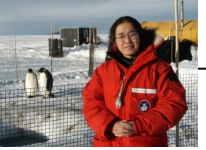
Temperature Measurement Techniques

- A direct measurement is to measure the velocity distribution and then take its statistical average as the definition of temperature. However, this is extremely difficult to do, so impractical.

Use temperature-dependent/sensitive effects or phenomena in *in-situ* measurements or remote sensing measurements.

- Temperature dependent & temperature sensitive effects or phenomena that can be used to measure temperatures – like expansion coefficient, resistivity, voltage, capacity, thermal radiation, etc., used in various forms of thermometers. These physical properties vary with temperature.

Many temperature measurement methods and instruments can be found today, all utilizing some physical properties or effects that vary with temperature. Most of them are for in-situ measurements, but some can be used in remote sensing.

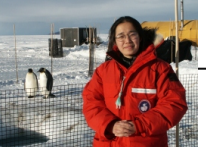


Temperature Measurement Techniques in Atmospheric Lidars

Use temperature-dependent/sensitive effects or phenomena

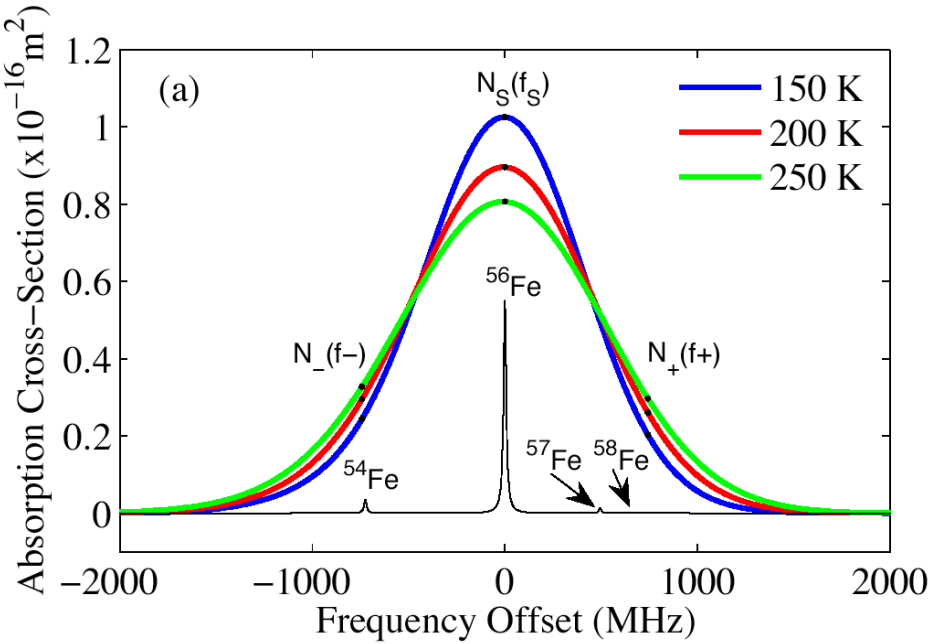
- Doppler Technique - Doppler broadening of radiation spectrum caused by thermal motions (not only for Fe, Na, and K etc. atomic absorption, but also for Rayleigh scattering, Raman scattering, and molecular absorption, as long as Doppler broadening dominate and can be detected)
- Boltzmann Technique - Boltzmann distribution of atomic/molecular populations on different energy levels under thermodynamic equilibrium (not only for Fe atomic absorption, but also for Raman scattering, molecular absorption, and airglow in optical remote sensing)
- Integration Technique (Rayleigh or Raman) - integration lidar technique using ideal gas law and assuming hydrostatic equilibrium (not only for modern lidar, but also for cw searchlight and rocket falling sphere - some way to measure atmosphere number density)

Each technique can be applied to various physical processes, such as atomic absorption or fluorescence, molecular absorption, Rayleigh scattering, and Raman scattering, etc.

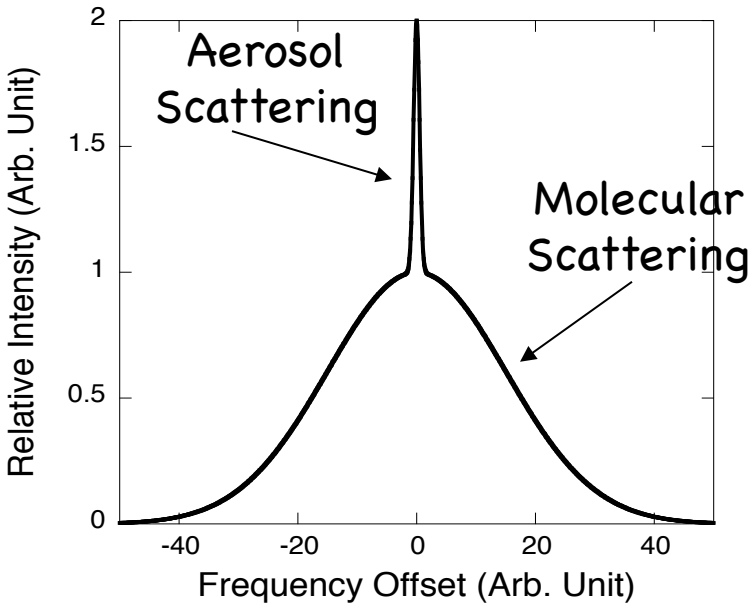


Overview: Doppler Technique

- Doppler broadening of radiation spectrum (absorption and scattering) is due to the thermal motions of atoms or molecules under thermodynamic equilibrium, whose distribution is governed by the Maxwellian velocity distribution law and strongly dependent on temperatures.



Atomic or Molecular Absorption Line

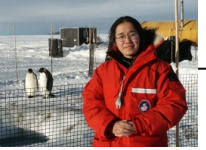


Rayleigh or Raman Scattering

$$\sigma_{rms} = \frac{\nu_0}{c}\sqrt{\frac{k_B T}{M}} = \frac{1}{\lambda_0}\sqrt{\frac{k_B T}{M}} = \sqrt{\frac{k_B T}{M\lambda_0^2}}$$

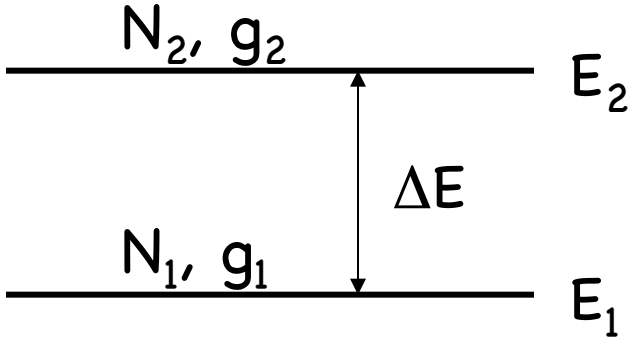
$$\sigma_{rms} = 2\nu_0 / c\sqrt{k_B T / M} = \frac{2}{\lambda_0}\sqrt{k_B T / M}$$

Doppler Spectrum (Doppler Broadening Width) ⇨ Temperature



Overview: Boltzmann Technique

- Boltzmann distribution is the law of particle (atom or molecule) population distributions according to energy levels and temperatures under thermodynamic equilibrium (Maxwell-Boltzmann distribution law), which is strongly temperature dependent.



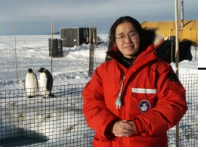
$$\frac{N_2}{N_1} = \frac{g_2}{g_1}\exp\left\{-\left(E_2 - E_1\right)/k_B T\right\}$$

$$T = \frac{\Delta E / k_B}{\ln\left(\frac{g_2}{g_1}\cdot\frac{N_1}{N_2}\right)}$$

$$\frac{N_k}{N} = \frac{g_k \exp(-E_k / k_B T)}{\sum_i g_i \exp(-E_i / k_B T)}$$

N_1 and N_2 – particle populations on energy levels E_1 and E_2
g_1 and g_2 – degeneracy for energy levels E_1 and E_2, $\Delta E = E_2 - E_1$
k_B – Boltzmann constant, T – Temperature, N – total population

Population Ratio ⇨ Temperature



Overview: Integration Technique

- Integration technique is to utilize the ideal gas law and hydrostatic equation to derive atmospheric temperatures from relative number density (i.e., number density ratio) if a seeding temperature is given.

Hydrostatic Equation

$$dP = -\rho g dz$$

+

Ideal Gas Law

$$P = \rho R T$$

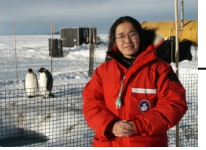
$$T(z) = T(z_o)\frac{\rho(z_o)}{\rho(z)} + \frac{1}{R}\int_z^{z_o} g(r)\frac{\rho(r)}{\rho(z)}dr$$

Seeding Temperature

Relative Density

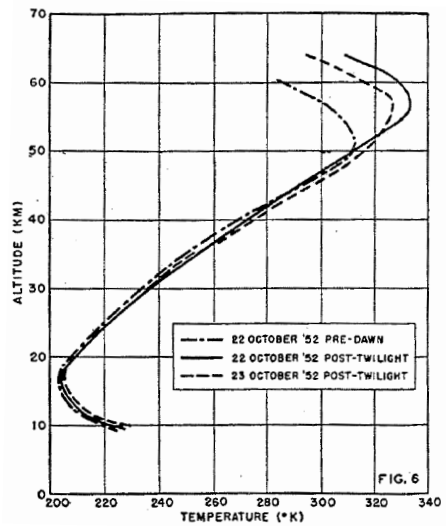
$T(z_0)$ - Seeding Temperature; ρ - number density
R - gas constant for dry air; g - gravitational acceleration

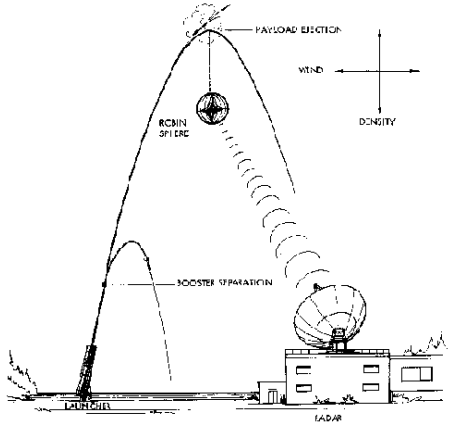
Number Density Ratio ⇨ Temperature
(lidar backscatter ratio at different altitudes)



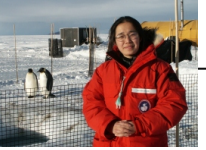
Integration Technique Principles
From Searchlight to Rayleigh, Raman & Falling Sphere

- Integration temperature technique relies on the assumptions of hydrostatic equilibrium equation and ideal gas law in atmosphere. It involves integrating the atmosphere relative density profile downward using a starting temperature at an upper altitude.
- It started with cw searchlight to measure stratospheric density thus deriving temperature in 1950s. The use of high power lasers with the Rayleigh lidar in the atmosphere region (30-100 km) free of aerosol and fluorescence was started in 1980.
- In the lower atmosphere where aerosol scattering contaminates Rayleigh scattering, Raman lidars were developed to measure atmosphere density from vibrational Raman scattering and then derive temperature below 30 km.
- Inflatable falling sphere provides high-precision atmosphere density thus temperature measurements.

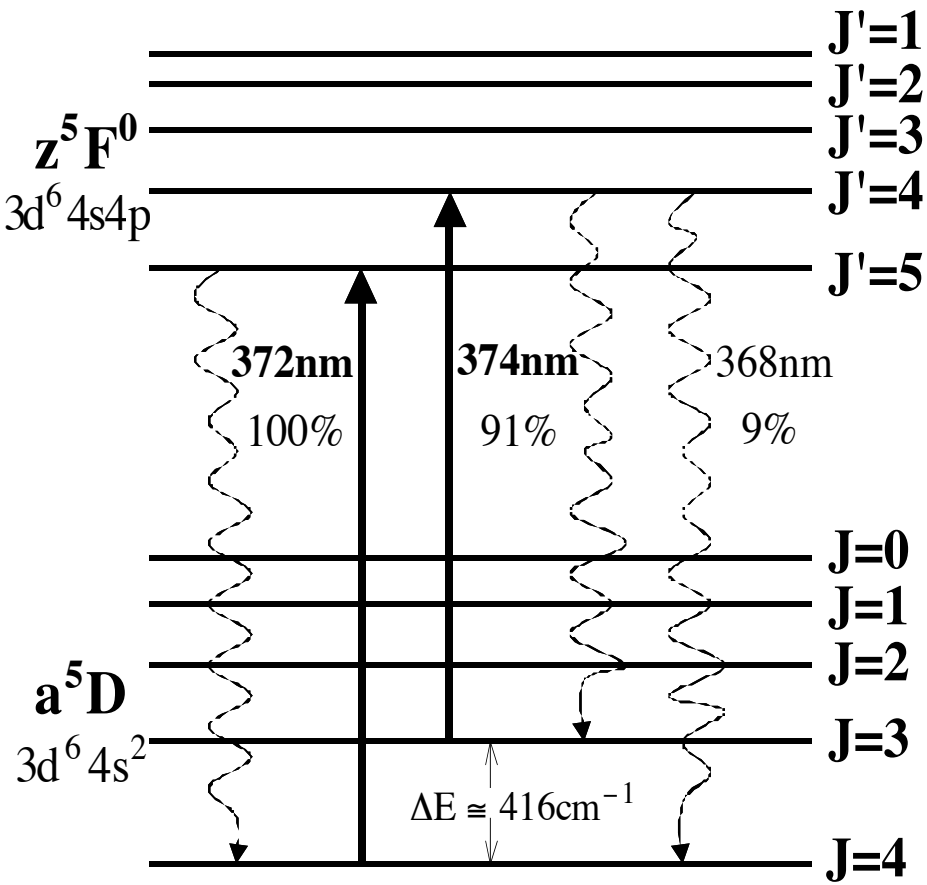




SPACE DATA CORPORATION Bollerman and Walker, 1968



Fe-Resonance Boltzmann Principle



Atomic Fe Energy Level

[Gelbwachs, 1994; Chu et al., 2002]

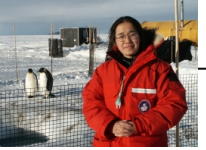
Maxwell-Boltzmann Distribution in Thermal-dynamic Equilibrium

$$\frac{P_2(J=3)}{P_1(J=4)} = \frac{\rho_{Fe(374)}}{\rho_{Fe(372)}} = \frac{g_2}{g_1} exp(-\Delta E / k_B T)$$

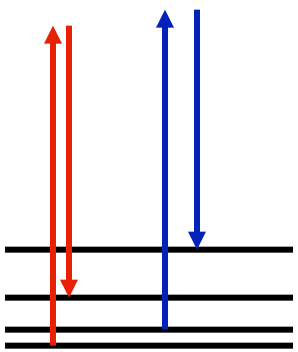
$$T = \frac{\Delta E / k_B}{ln\left(\frac{g_2}{g_1} \cdot \frac{P_1}{P_2}\right)}$$

P_1, P_2 -- Fe populations
g_1, g_2 -- Degeneracy
k_B -- Boltzmann constant
T -- Temperature

Population Ratio ⇨ Temperature



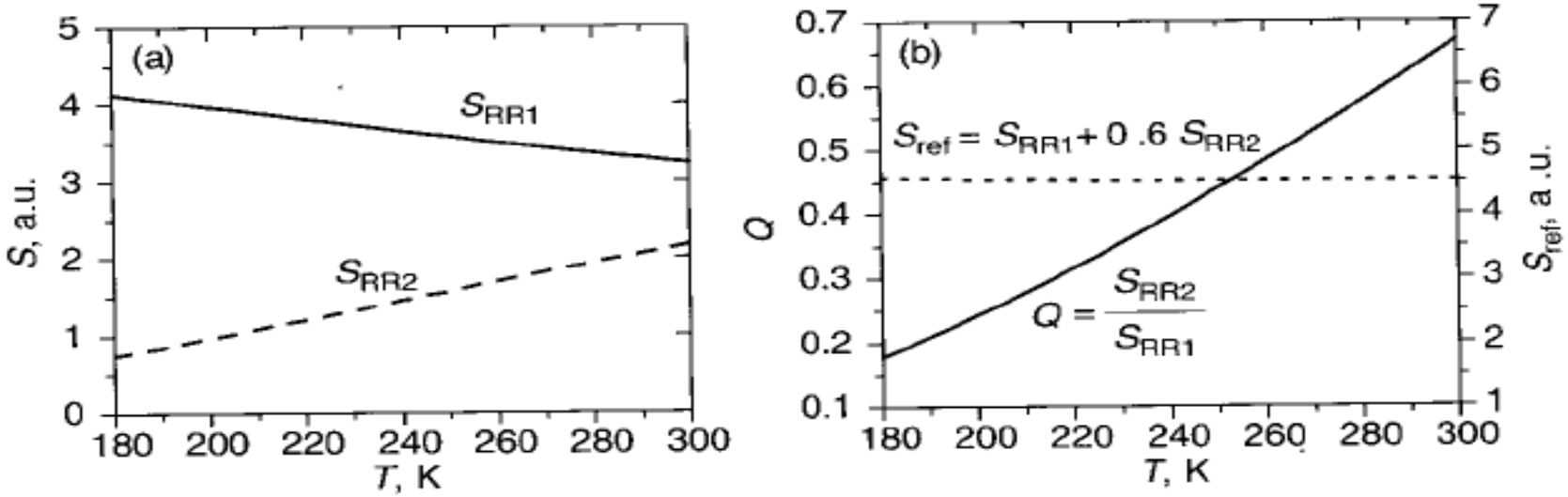
Rotational-Raman Boltzmann Principe



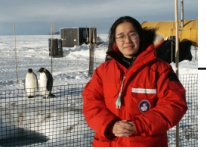
V=0, J=0

$$Q(T) = \frac{\sum_{i=O_2,N_2} \sum_{J_i} \tau_{RR2}(J_i)\eta_i \left(\frac{d\sigma}{d\Omega}\right)_{\pi}^{RR,i}(J_i)}{\sum_{i=O_2,N_2} \sum_{J_i} \tau_{RR1}(J_i)\eta_i \left(\frac{d\sigma}{d\Omega}\right)_{\pi}^{RR,i}(J_i)}$$

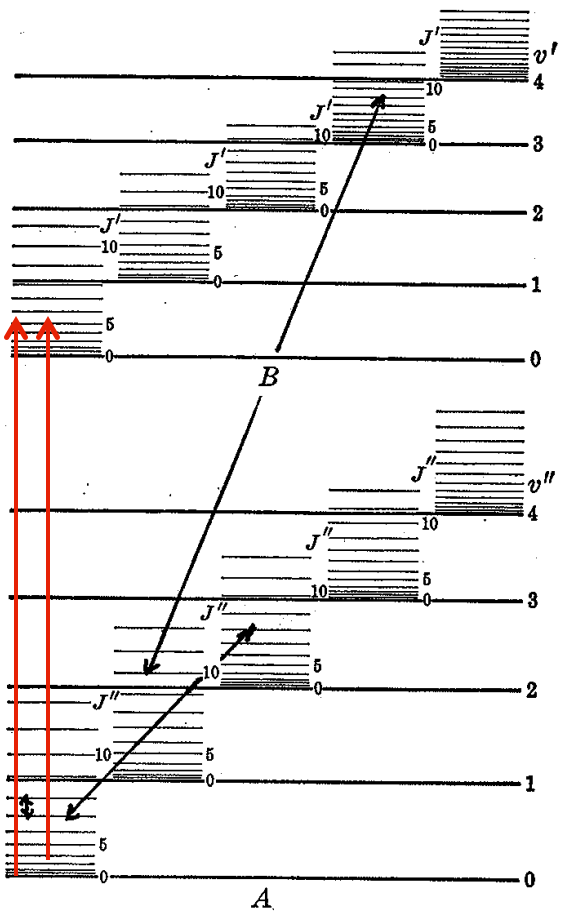
where τ is the receiver transmission at RR line, η is the relative volume abundance of N_2 & O_2.



- Temperature can be derived from the ratio of two pure rotational Raman line intensities, which have opposite temperature dependence due to the Boltzmann distribution of populations on energy levels.

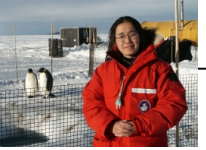


Absorption or DIAL Boltzmann Principle



- For molecules that have suitable absorptions originating from ground states or near ground states, the population ratis of different energy levels can be measured via detecting the molecular absorptions that are proportional to the populations on corresponding energy levels.
- It may be necessary to use DIAL (differential absorption) technique to measure the molecular absorptions at different wavelengths that correspond to different energy levels.
- Then temperature can be inferred from the population ratios using the Boltzmann distribution law.

- Temperature can be derived from the ratio of two molecular absorption line intensities, which is proportional to the ratio of populations on the corresponding initial energy levels.



Doppler Technique to Measure Temperature and Wind

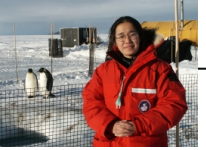
- Doppler effect is commonly experienced by moving particles, such as atoms, molecules, and aerosols. It is the apparent frequency change of radiation that is perceived by the particles moving relative to the source of the radiation. This is called Doppler shift or Doppler frequency shift.
- Doppler frequency shift is proportional to the radial velocity along the line of sight (LOS) of the radiation -

$$\omega = \omega_0 - \vec{k} \cdot \vec{v}$$

$$\Delta\omega = \omega - \omega_0 = -\vec{k} \cdot \vec{v} = -\omega_0 (v/c)\cos\theta$$

$$\Delta\nu = -\nu_0 (v/c)\cos\theta = -(v/\lambda_0)\cos\theta$$

where ω_0 is the radiation frequency at rest, ω is the shifted frequency, k is the wave vector of the radiation ($k=2\pi/\lambda$), and v is the particle velocity.



Doppler Technique

- Due to particles' thermal motions in the atmosphere, the distribution of perceived frequencies for all particles mirrors their velocity distribution. According to the Maxwellian velocity distribution (Gaussian),

$$P(v_R \rightarrow v_R + dv_R) \propto \exp\left(-Mv_R^2/2k_BT\right)dv_R$$

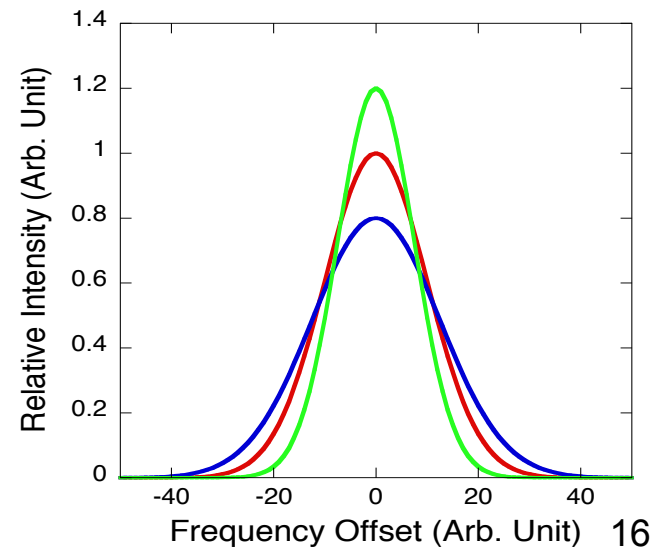
$$\omega = \omega_0 + \vec{k}\cdot\vec{v} = \omega_0\left(1+\frac{v_R}{c}\right) \Rightarrow v_R = \frac{\omega-\omega_0}{\omega_0/c} = \frac{\nu-\nu_0}{\nu_0/c}$$

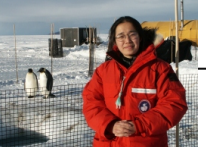
- Substituting v_R into the probability distribution, we obtain the power spectral density distribution (i.e., intensity versus the perceived frequency by moving particles) as a Gaussian lineshape,

$$I \propto \exp\left(-\frac{M(\nu-\nu_0)^2}{2k_BT(\nu_0/c)^2}\right)(c/\nu_0)d\nu$$

- This is called Doppler broadening of a line. The peak is at $\omega = \omega_0$ and the rms width is

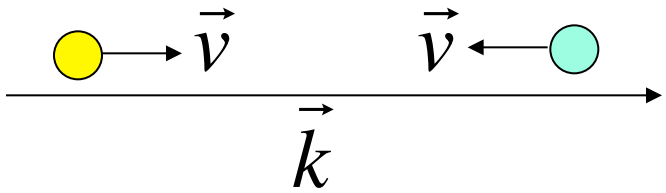
$$\sigma_{rms} = \frac{\nu_0}{c}\sqrt{\frac{k_BT}{M}} = \frac{1}{\lambda_0}\sqrt{\frac{k_BT}{M}}$$





Doppler Shift in Absorption

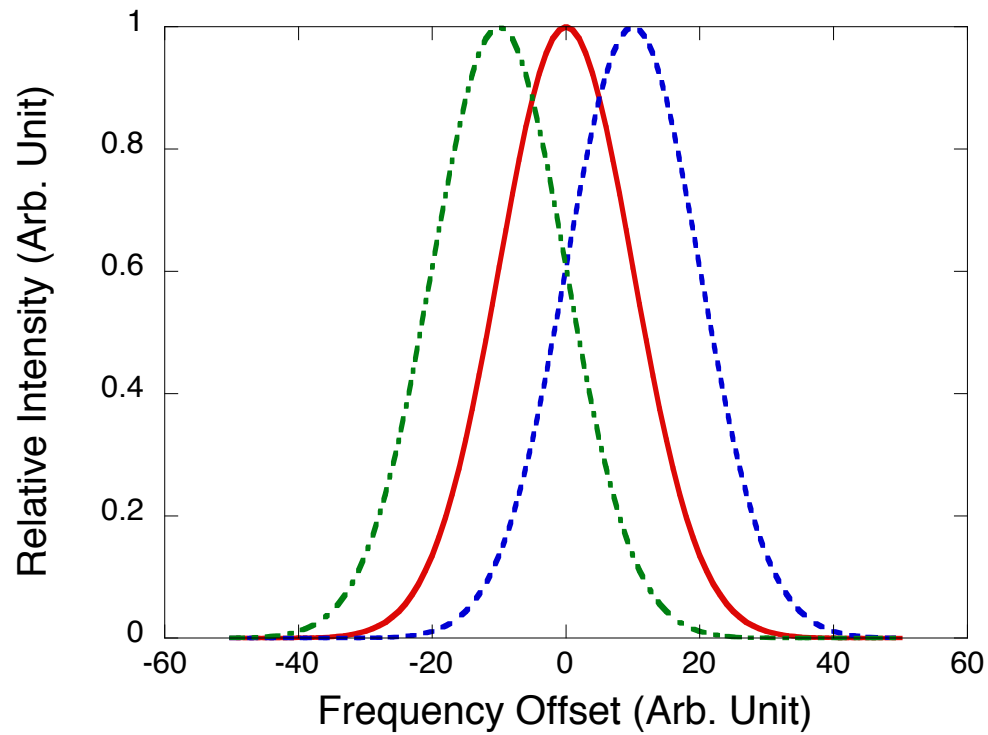
$$\Delta\omega = \omega - \omega_0 = -\vec{k}\cdot\vec{v} = -\omega_0 \frac{v\cos\theta}{c} \qquad (12.13)$$



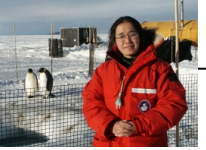
Emitter and receiver move towards each other:

-Blue shift in perceived radiation frequency

-Red shift in absorption peak frequency



- The velocity measurements of lidar, radar, and sodar all base on the Doppler shift principle !



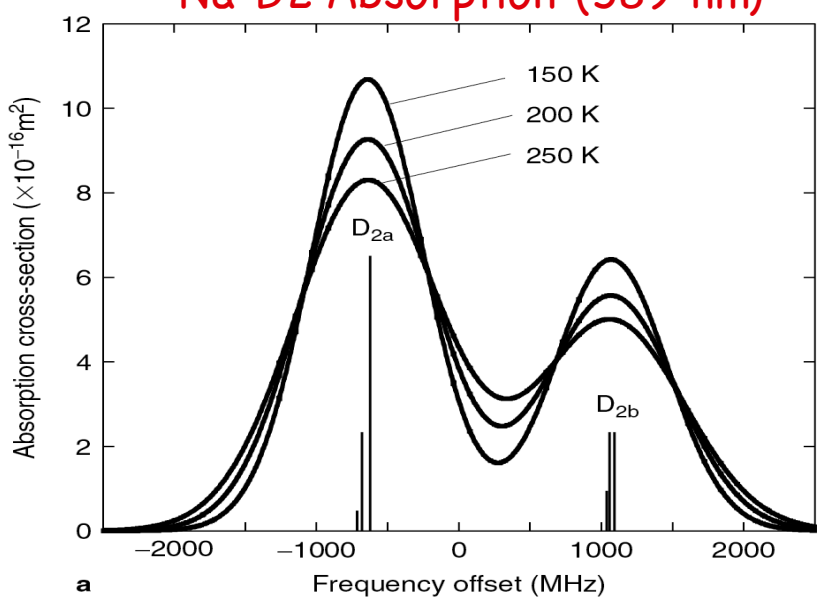
Doppler Broadening in Resonance Absorption Lines

$$\sigma_{rms} = \frac{\nu_0}{c}\sqrt{\frac{k_B T}{M}} = \frac{1}{\lambda_0}\sqrt{\frac{k_B T}{M}}$$

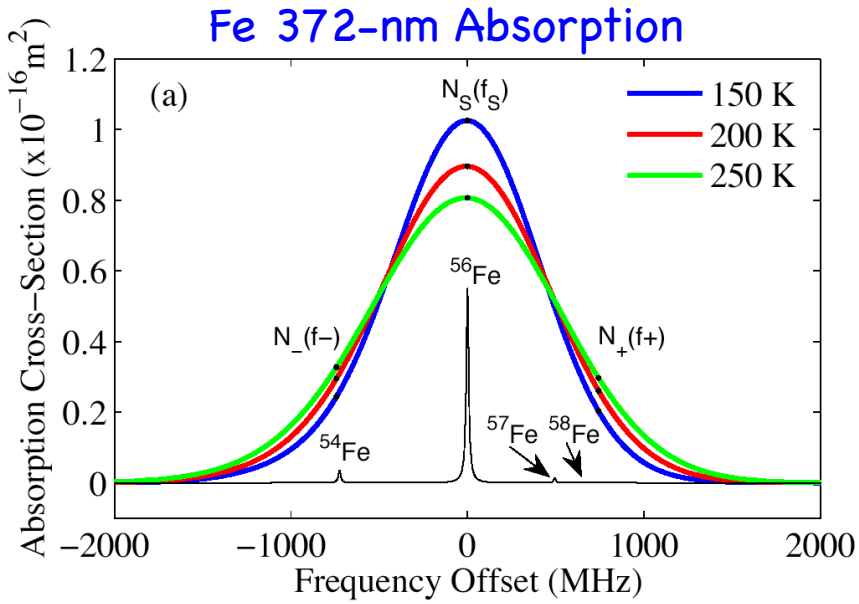
T ↗ ⇨ σ_{rms} ↗

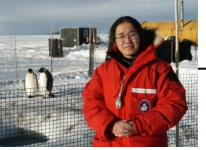
M ↗ ⇨ σ_{rms} ↘

Na D2 Absorption (589 nm)



Fe 372-nm Absorption





Doppler Shift and Broadening in Resonance Fluorescence

- When an atom emits a resonance fluorescence photon, the photon has Doppler shift relative to the center freq. of the atomic absorption line as

$$\omega = \omega_0 + \vec{k}\cdot\vec{v} = \omega_0\left(1+\frac{v_R}{c}\right) \Rightarrow v_R = \frac{\omega-\omega_0}{\omega_0/c} = \frac{\nu-\nu_0}{\nu_0/c}$$

- According to the Maxwellian velocity distribution, the relative probability that an atom/molecule in a gas at temperature T has its velocity component along the line of sight between v_R and v_R+dv_R is

$$P(v_R \rightarrow v_R + dv_R) \propto \exp\left(-Mv_R^2/2k_BT\right)dv_R$$

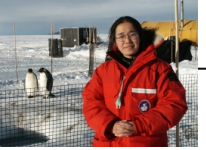
- Substitute the v_R equation into the Maxwellian distribution,

$$I \propto \exp\left(-\frac{M(\nu-\nu_0)^2}{2k_BT(\nu_0/c)^2}\right)(c/\nu_0)d\nu$$

- Therefore, the rms width of the Doppler broadening is

$$\sigma_{rms} = \nu_0/c\sqrt{k_BT/M} = \frac{1}{\lambda_0}\sqrt{k_BT/M}$$

1 time



Doppler Shift in Rayleigh Scattering

- Refer to textbook 5.2.2.4 Lidar wind vs radar wind measurements

Momentum Conservation $m\vec{v}_1 + \hbar\vec{k}_1 = m\vec{v}_2 + \hbar\vec{k}_2$

Energy Conservation $\frac{1}{2}mv_1^2 + \hbar\omega_1 = \frac{1}{2}mv_2^2 + \hbar\omega_2$

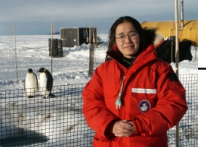
$$\boxed{\omega_1 = \omega_2 + \vec{k}_1 \cdot \vec{v}_1 - \vec{k}_2 \cdot \vec{v}_2 + \frac{\hbar k_1^2}{2m} - \frac{\hbar k_2^2}{2m}}$$

- For Rayleigh or radar backscatter signals, we have

$$\vec{k}_2 \approx -\vec{k}_1 \qquad \vec{v}_2 \approx \vec{v}_1$$

- The frequency shift for Rayleigh or radar backscattering is

$$\boxed{\Delta\omega_{Rayleigh,backscatter} = \omega_2 - \omega_1 = -2\vec{k}_1 \cdot \vec{v}_1}$$



Doppler Broadening in Rayleigh Scatter

- To derive the Doppler broadening, let's write the Doppler shift as

$$\omega = \omega_0\left(1 - \frac{2v_R}{c}\right) \Rightarrow v_R = \frac{\omega_0 - \omega}{2\omega_0/c} = \frac{\nu_0 - \nu}{2\nu_0/c}$$

- According to the Maxwellian velocity distribution, the relative probability that an atom/molecule in a gas at temperature T has its velocity component along the line of sight between v_R and v_R+dv_R is

$$P(v_R \to v_R + dv_R) \propto \exp\left(-Mv_R^2/2k_BT\right)dv_R$$

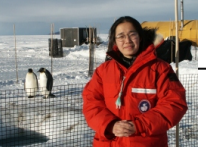
- Substitute the v_R equation into the Maxwellian distribution,

$$I \propto \exp\left(-\frac{M(\nu_0 - \nu)^2}{2k_BT(2\nu_0/c)^2}\right)(c/2\nu_0)d\nu$$

- Therefore, the rms width of the Doppler broadening is

$$\sigma_{rms} = 2\nu_0/c\sqrt{k_BT/M} = \frac{2}{\lambda_0}\sqrt{k_BT/M}$$

2 times !



Doppler Effect in Rayleigh Scattering

- In the atmosphere when aerosols present, the lidar returns contains a narrow spike near the laser frequency caused by aerosol scattering riding on a Doppler broadened molecular scattering profile.

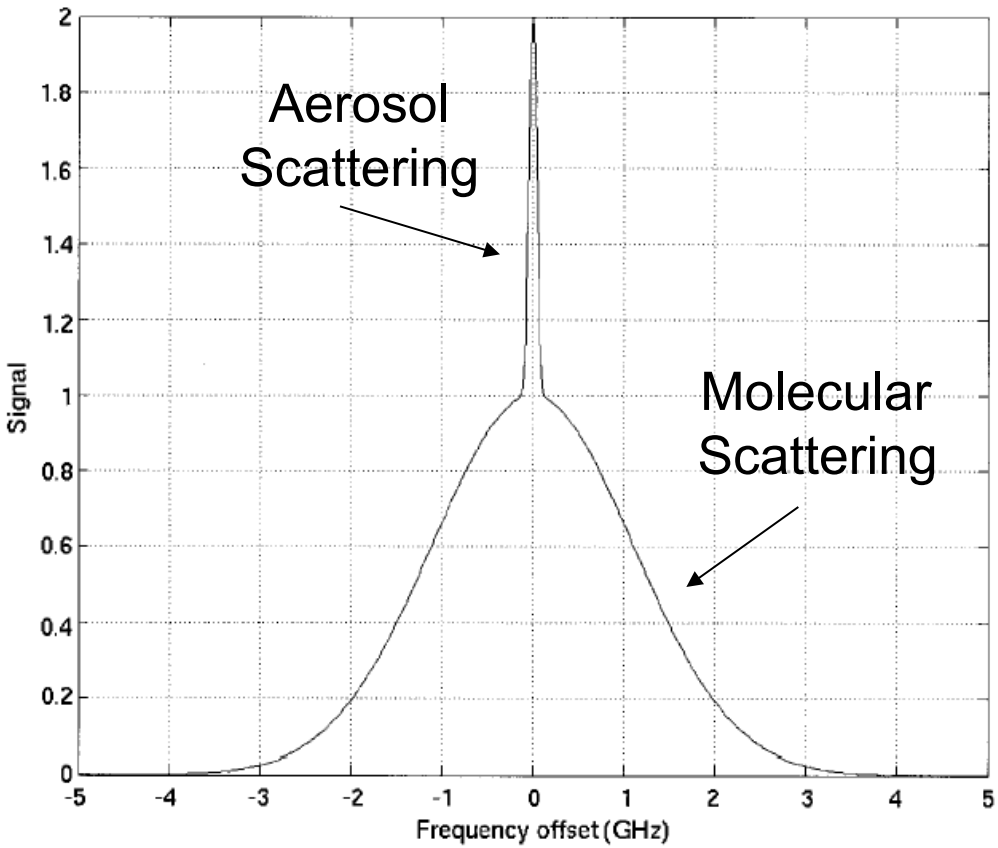
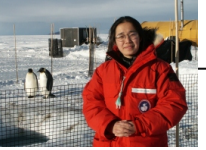


Fig. 5.1. Spectral profile of backscattering from a mixture of molecules and aerosols for a temperature of 300 K. The spectral width of the narrow aerosol return is normally determined by the line width of the transmitting laser.

At T = 300 K, the Doppler broadened FWHM for Rayleigh scattering is 2.58GHz, not 1.29GHz.
Why?

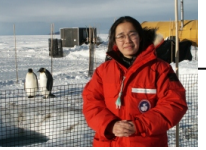
Because Rayleigh backscatter signals have 2 times of Doppler shift!

Courtesy of Dr. Ed Eloranta
University of Wisconsin



Various Physical Interactions and Techniques are Applied to Doppler Tech

- When resonance absorption and fluorescence is available (not quenched), the resonance Doppler lidar can be employed to probe Doppler broadening and Doppler shift. It can be atomic resonance fluorescence or molecular resonance fluorescence in the upper atmosphere.
- If molecular absorption is available, then DIAL lidar can be employed to infer the Doppler broadening in molecular absorption for temperature. This is doable in the lower atmosphere.
- Rayleigh scattering experiences Doppler broadening, so it can be measured using various techniques (e.g., edge filter, interferometers, etc.) to infer the temperature.
- High-spectral-resolution lidar (HSRL) can help remove aerosol contamination to reveal Doppler broadening for temperature.
- Vibrational-rotational Raman scattering should experience similar Doppler broadening as Rayleigh scattering, but it has shifted frequencies of return signals, which may help avoid the contamination of aerosol scattering to Rayleigh scattering.



Summary

- Temperature is a measure of the statistical average kinetic energy of particles (atoms or molecules) under thermodynamic equilibrium established by collisions among particles.
- The key point to measure temperature is to find and use temperature-dependent effects and phenomena to make measurements, rather than measuring the velocity distribution of particles and then taking the statistical average.
- Atmospheric lidars mainly utilize three physical effects to measure temperatures remotely: Doppler technique, Boltzmann technique, and integration technique. Each of these techniques can have various realizations through measuring the effects in atomic absorption or fluorescence, in molecular absorption, in Rayleigh scattering, or in Raman scattering, etc., leading to various names under the same effects.
  - Doppler technique can have resonance Doppler, Rayleigh Doppler, DIAL Doppler, Raman Doppler, etc.
  - Boltzmann technique can have Fe-resonance Boltzmann, rotational-Raman Boltzmann, DIAL Boltzmann, etc.
  - Integration technique can be applied to falling sphere, search light, Rayleigh and Raman lidars.