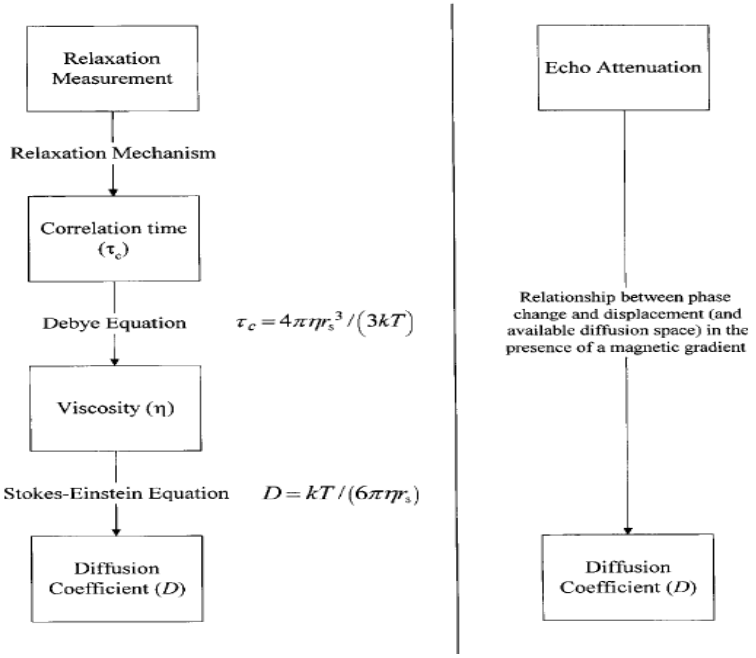
Diffusion Coefficient Measurement by Nuclear Magnetic Resonance

Two Kinds of Diffusion Motion Measurement by NMR

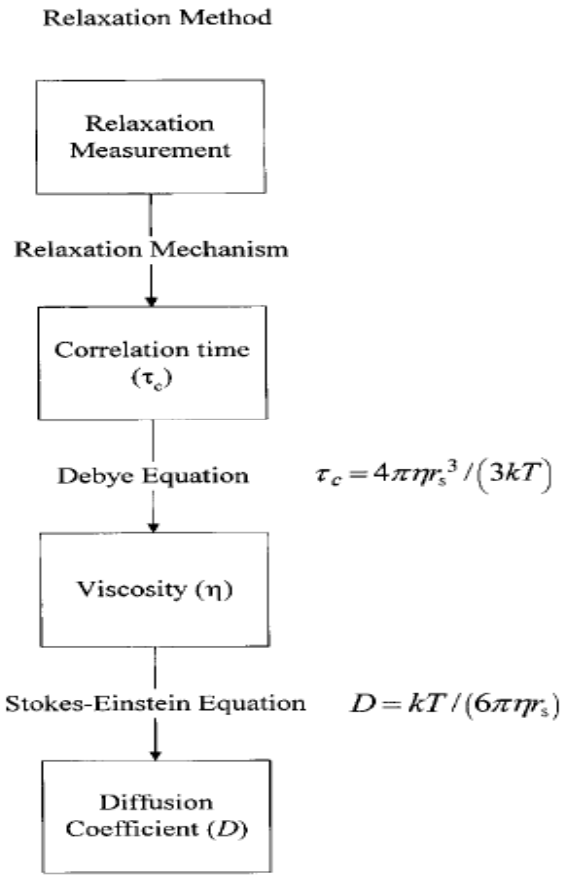
	Relaxation Method	Pulsed Field Gradient Method
Measured Time Scale	ps to ns	ms to s
Correspondence Motion	Rotational diffusion motion	Translational diffusion motion



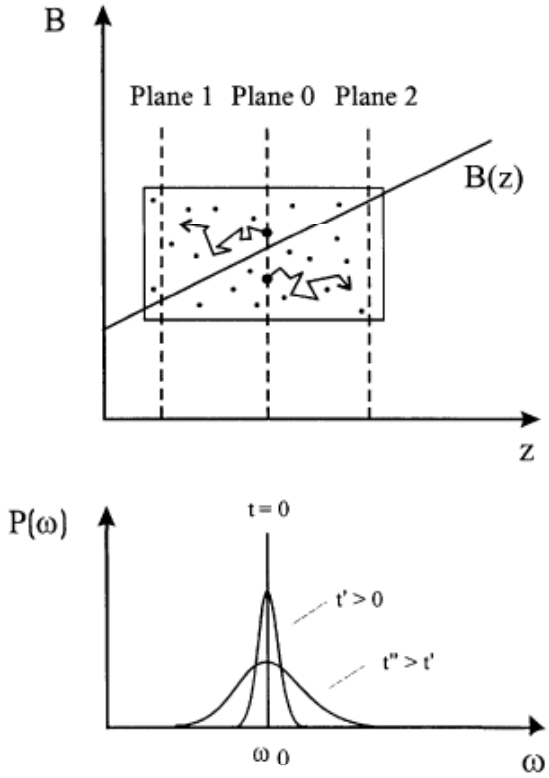
Two Kinds of Diffusion Motion Measurement by NMR

Assumptions

1. Basic Information – relaxation mechanism
2. Molecular Shape
3. Relative Size of Molecules
4. Absolute Size of Prove Molecule

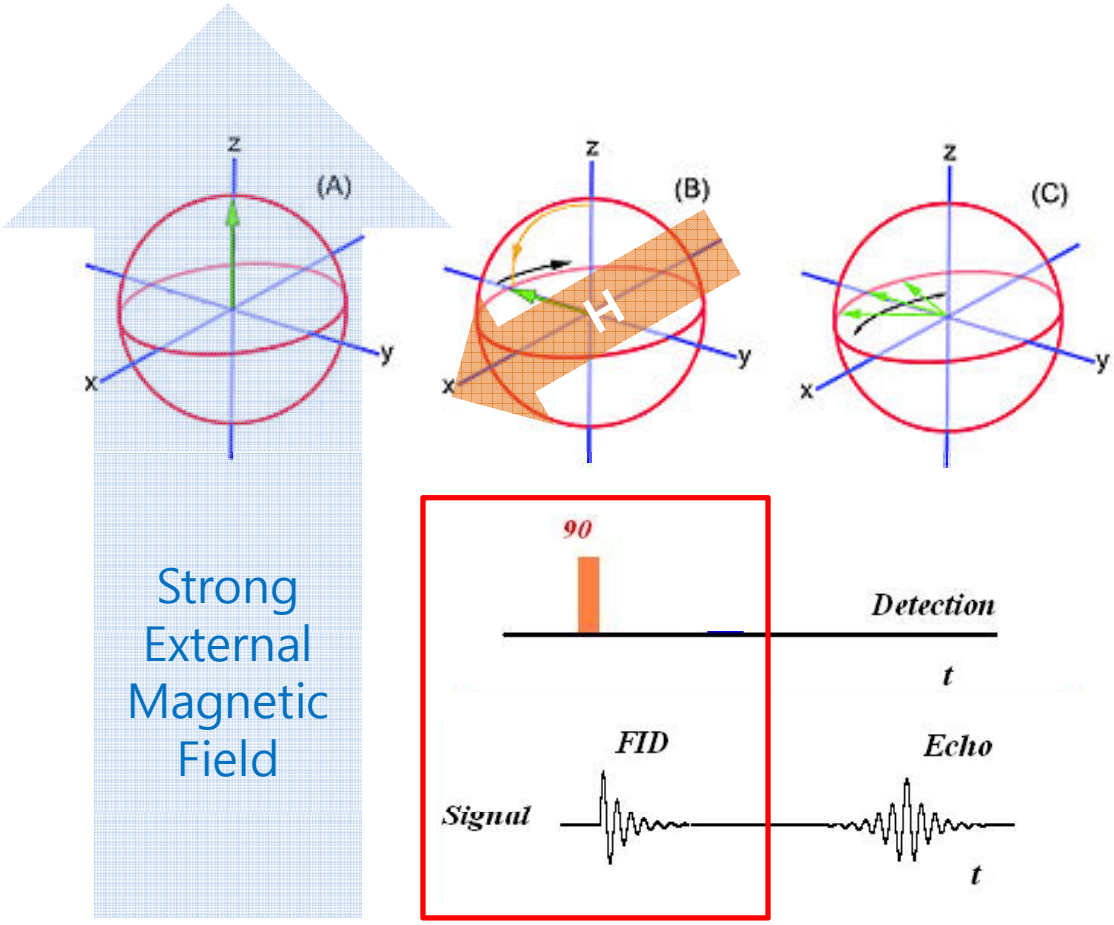


Basic Idea



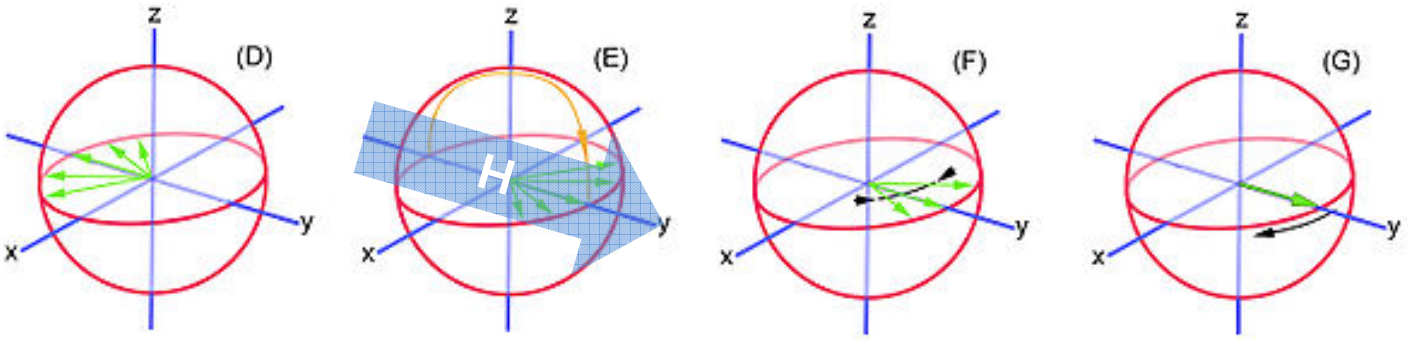
Diffusion Motion makes the Spectral Broadening

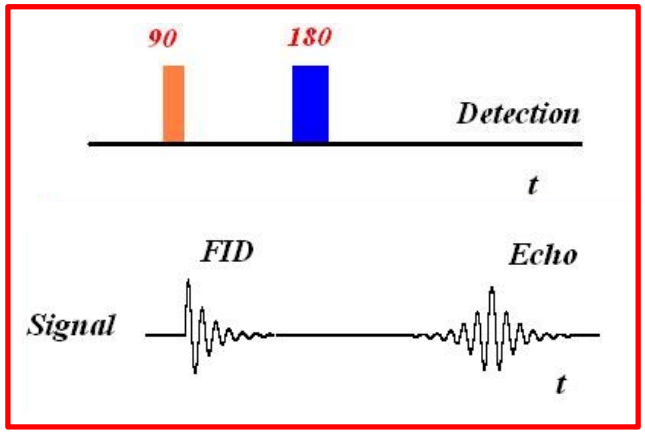
Spin Echoes (1) - dephasing



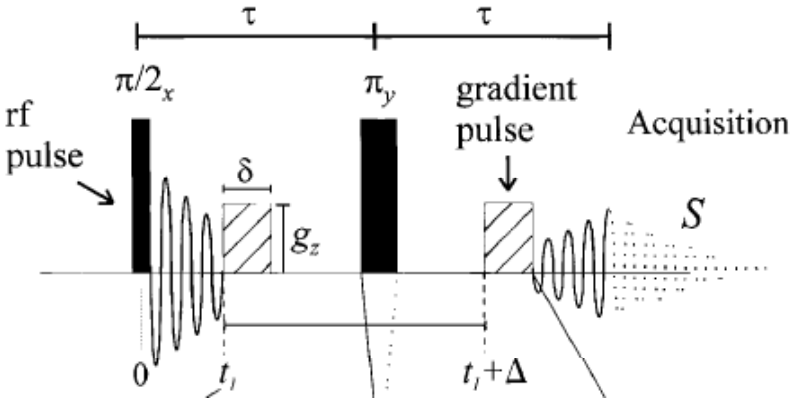
The inhomogeneous field makes the fanning out in (c)

Spin Echoes (2) - refocusing





Effect of Diffusion



$$\phi(t) = \gamma B_0 t + \gamma \int_0^t g(t')z(t')dt$$

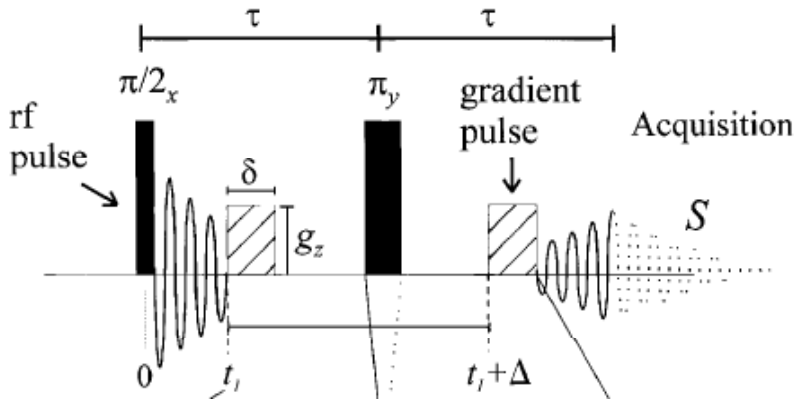
$$\phi(t) = \gamma B_0 t + \gamma g \int_0^t z(t')dt$$

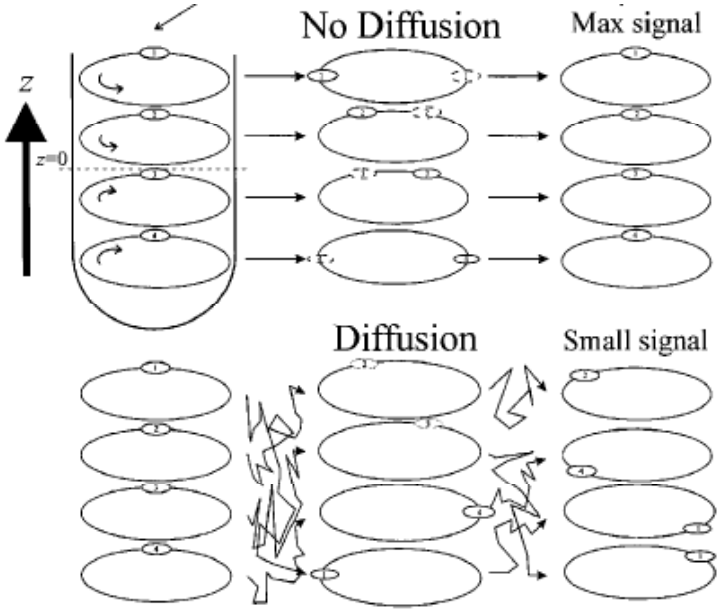
$$\phi_i(2\tau) = (\gamma B_0 t + \gamma g \int_{t_1}^{t_1+\delta} z(t)dt) - (\gamma B_0 t + \gamma g \int_{t_1+\Delta}^{t_1+\Delta+\delta} z(t')dt')$$

$$\phi_i(2\tau) = \gamma g (\int_{t_1}^{t_1+\delta} z(t)dt - \int_{t_1+\Delta}^{t_1+\Delta+\delta} z(t')dt')$$

$$S(2\tau) = C \int_{-\infty}^{\infty} P(\phi, 2\tau)\cos\phi d\phi$$

Effect of Diffusion





$$\phi(t) = \gamma B_0 t + \gamma \int_0^t g(t')z(t')dt$$

$$\phi(t) = \gamma B_0 t + \gamma g \int_0^t z(t')dt$$

Effect of Diffusion

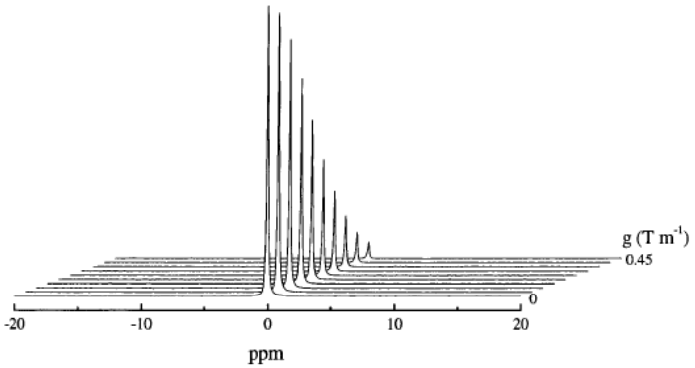


Figure 3 ^{13}C-PFG NMR spectra of a sample of $^{13}CCl_4$. The spectra were acquired at 303 K with Δ 100 ms, δ 4 ms, and *g* ranging from 0 to 0.45 T m $^{-1}$ in 0.05-T m $^{-1}$ increments. The spectra are presented in phase-sensitive mode with a line broadening of 5 Hz. As the intensity of the gradient increases, the echo intensity decreases due to the effects of diffusion.

$$S(2\tau) = S(0)\exp(2\tau / T_2)\, f(D)$$

$$S(2\tau) = S(0)\exp(2\tau / T_2)\exp(2\gamma^2 D g^2 \tau^2 / 3)$$