

Homework set 2/3, deadline: 11 January 2025, 12:00 Tel Aviv time

Solutions to be submitted by email to ilya.kuprov@weizmann.ac.il in any reasonable format.

1. Use Fourier transform (from 0 to infinity with respect to time) of both sides to convert the differential form of Schrödinger's equation in the time domain:

$$\frac{d}{dt}\psi(t) = -i\hat{H}\psi(t), \quad \psi(0) = \psi_0$$

into an algebraic form in the frequency domain. Assume that the Hamiltonian does not depend on time and use integration by parts. Given the availability of fast Fourier transform, which representation of Schrödinger's equation is easier to deal with computationally? [15 marks]

2. Use the following definition of delta-function:

$$\delta(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t} d\omega$$

and Euler's relations for sine and cosine:

$$\sin(\omega t) = \frac{e^{i\omega t} - e^{-i\omega t}}{2i}, \quad \cos(\omega t) = \frac{e^{i\omega t} + e^{-i\omega t}}{2}$$

to demonstrate that Fourier transforms of $\sin(\omega t)$ and $\cos(\omega t)$ are linear combinations of delta functions centred at $\pm\omega$ in the frequency domain. How would these Fourier transforms look in practical NMR spectroscopy, where sine and cosine functions decay with time? [20 marks]

3. What would have happened if Otto Stern and Walther Gerlach had used, in their famous 1922 experiment, instead of electrically neutral silver atoms:
 - (a) neutral ytterbium atoms? [5 marks]
 - (b) neutral thulium atoms? [5 marks]
 - (c) singly charged silver ions? [5 marks]
4. Draw the effective magnetic field vector in the rotating frame for protons ($\gamma = 42.6 \times 10^6$ Hz/T) during an X-pulse of 1 mT amplitude, at a static magnetic field of 14.1 T, if:
 - (a) the pulse frequency is on resonance [5 marks]
 - (b) the pulse frequency is 50 kHz above resonance [5 marks]
 - (c) the pulse frequency is 50 kHz below resonance [5 marks]

5. ^{195}Pt chemical shifts cover about 15000 ppm, ranging from +11840 ppm for $[\text{PtF}_6]^{2-}$ to -3000 ppm for Pt(II) complexes. The magnetogyric ratio of ^{195}Pt is $9.29 \times 10^6 \text{ Hz/T}$.
- (a) What is the spin precession frequency at a magnetic field of 11.7 T? [5 marks]
 - (b) At 11.7 T, what is the frequency range covered by the above chemical shifts? [5 marks]
 - (c) Why is it sometimes possible to use ^{13}C NMR probes for ^{195}Pt experiments? [5 marks]
6. Explain the mathematical (Hamiltonian) and the experimental (appearance of the spectrum) difference between strong and weak J -coupling. For the following systems, give a rational explanation for the type of the expected J -coupling.
- (i) ^1H - ^{19}F J -coupling in zero magnetic field. [5 marks]
 - (ii) ^1H - ^{13}C J -coupling in a 14.1 Tesla magnet. [5 marks]
 - (iii) ^1H - ^1H J -coupling in cis-1-chloro-2-fluoroethylene in a 14.1 Tesla magnet. [5 marks]
 - (iv) ^1H - ^1H J -coupling in cis-1-chloro-2-fluoroethylene in a 50000 Tesla magnet. [5 marks]