M520 Non-Relativistic Quantum Mechanics

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Homework Assignment 3

DUE: Monday 7 August 2023

55+10 points

- 1. Spreading of a free wave packet (10 points) C-T $L_{\rm III}$ 4.
- 2. Particle subjected to a constant force (10 points). C-T $L_{\rm III}$ 5.
- 3. Virial theorem (5 points). C-T L_{III} 10 (a) only!
- 4. (10 points). C-T $J_{\rm IV}$ 3.
- 5. Evolution operator of a spin 1/2(10 points). C-T $J_{\rm IV}$ 5.

6. Nuclear Magnetic Resonance (10+10 points).

Consider a spin-1/2 particle in a constant external field $\mathbf{B} = B_0 \hat{\mathbf{e}}_z$ under the influence of some time-dependent Hamiltonian $\widehat{W}(t)$, leading to the total Hamiltonian

$$\widehat{H}(t) = \widehat{H}_0 + \widehat{W}(t); \tag{1}$$

 $\widehat{H}_0 = -\mu \cdot \mathbf{B} = \gamma B_0 \widehat{S}_z = -\hbar \Omega \, \widehat{\sigma}_z / 2$, where $\Omega = \gamma B_0$ is the Larmor frequency. In order to study the dynamics governed by the time-dependent part, it is useful to move into the rotating frame of reference in which the spin no longer precesses about the z axis. Let $\widehat{U}_0 = \exp(i\Omega \widehat{\sigma}_z t / 2)$ be the free time-evolution operator, and define

$$|\psi_I(t)\rangle := \widehat{U}_0^{\dagger}(t,0) |\psi(t)\rangle, \qquad \qquad \widehat{H}_I(t) := \widehat{U}_0^{\dagger}(t,0)\widehat{W} \,\widehat{U}_0(t,0).$$
 (2)

The subscript I indicates that we are in the *interaction picture* (also known as the *Dirac picture*) in which both states and operators evolve in time.

(a) Show that the Schrödinger equation in the interaction picture takes on the familiar form

$$i\hbar \frac{d}{dt} |\psi_I(t)\rangle = \hat{H}_I(t) |\psi_I(t)\rangle.$$
 (3)

(b) Show that

$$\widehat{U}_{0}^{\dagger}\widehat{\sigma}_{z}\widehat{U}_{0} = \widehat{\sigma}_{z},
\widehat{U}_{0}^{\dagger}\widehat{\sigma}_{x}\widehat{U}_{0} = \cos(\Omega t)\widehat{\sigma}_{x} + \sin(\Omega t)\widehat{\sigma}_{y},
\widehat{U}_{0}^{\dagger}\widehat{\sigma}_{y}\widehat{U}_{0} = \cos(\Omega t)\widehat{\sigma}_{y} - \sin(\Omega t)\widehat{\sigma}_{x}.$$
(4)

Since any arbitrary $\widehat{W}(t)$ can be decomposed in the Pauli basis

$$\widehat{W}(t) = A_0 \widehat{1} + A_x \widehat{\sigma}_x + A_y \widehat{\sigma}_y + A_z \widehat{\sigma}_z, \tag{5}$$

we have that

$$\widehat{H}_I(t) = A_0 \widehat{1} + \left[A_x \cos(\Omega t) - A_y \sin(\Omega t) \right] \widehat{\sigma}_x + \left[A_x \sin(\Omega t) + A_y \cos(\Omega t) \right] \widehat{\sigma}_y + A_z \widehat{\sigma}_z. \tag{6}$$

If the Schrödinger-picture Hamiltonian is constant or varies slowly with time, the $\hat{\sigma}_x$ and $\hat{\sigma}_y$ terms in (6) will oscillate rapidly around zero, and thus the effect of these terms will be canceled out on average, leaving the net effect in the rotating frame being just an extra precession about the z axis.

(c) Now consider a specific oscillatory Hamiltonian

$$\widehat{W}(t) = \cos(\Omega' t - \phi)\widehat{\sigma}_x - \sin(\Omega' t - \phi)\widehat{\sigma}_y,\tag{7}$$

which could have been turned on by shining a circularly-polarized light onto the spin-1/2 particle. Use (6) to write down the interaction-picture Hamiltonian $\hat{H}_I(t)$. You can ignore the identity component $A_0\hat{\mathbb{I}}$, since it only contributes an overall global phase. Discuss what happens in the rotating frame if $\Omega - \Omega'$ is close to zero.

4(d) is an optional bonus problem.

(d) We can use this phenomenon of *nuclear magnetic resonance* to generate an arbitrary rotation of the quantum state of the spin-1/2 particle. Suppose that Ω' exactly matches the Larmor frequency: $\Omega - \Omega' = 0$. Describe how one would generate an arbitrary Z rotation in the rotating frame using a time-sequence of Hamiltonians of the form (7) with varying values of ϕ .

The following matrix forms may be helpful:

$$\widehat{R}_{x}(\theta) = e^{-i\theta\widehat{\sigma}_{x}/2} = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & -i\sin\left(\frac{\theta}{2}\right) \\ -i\sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{pmatrix}, \tag{8}$$

$$\widehat{R}_{y}(\theta) = e^{-i\theta\widehat{\sigma}_{y}/2} = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & -\sin\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{pmatrix},\tag{9}$$

$$\widehat{R}_z(\theta) = e^{-i\theta\widehat{\sigma}_z/2} = \begin{pmatrix} e^{-i\theta/2} & 0\\ 0 & e^{i\theta/2} \end{pmatrix}. \tag{10}$$

Magnetic Resonance Imaging (MRI) is a technique based on NMR that allows us to distinguish various kinds of tissues in the human body. In a typical MRI machine, the magnetic field's magnitude B_0 is a few Tesla, and radio-frequency pulses (with frequencies of the order of one to several hundred megahertz) are used to match the Larmor frequency. The actual mechanism responsible for MRI signals that one reads out is *decoherence*: non-unitary time evolutions that take pure quantum states to mixed quantum states.