Quantum Mechanics I, Sheet 10, Spring 2013

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I. INTERACTION PICTURE

The Heisenberg picture considered in sheet 9 allows one to transfer the time dependence from the wave function to operators. This is often convenient because this provides a way to evaluate the evolution of an operator by calculating the commutator with the Hamiltonian.
However, when a Hamiltonian consists of two parts one of which can be solved exactly it can be handy to split the time dependence between operators and the wave function in such a way that the "easy" part of the Hamiltonian determines the time dependence of operators, while for the "difficult" part we follow the evolution of the wave function in the same way as in the Schrödinger picture.
Consider a Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{W},$$

such that the spectrum of $\hat{H}_0$ can be found exactly, and $\hat{H}_0$, $\hat{W}$ do not generally commute. Usually, $\hat{W}$ represents an interaction part of the total Hamiltonian.
The interaction picture is defined by the following unitary transformation:

$$\begin{aligned} |\Phi(t)\rangle &= e^{\frac{i}{\hbar}\hat{H}_0 t} \, |\Psi(t)\rangle \, , \\ \hat{A}_I(t) &= e^{\frac{i}{\hbar}\hat{H}_0 t} \hat{A} e^{-\frac{i}{\hbar}\hat{H}_0 t}. \end{aligned}$$

1. Prove that if $|\Psi(t)\rangle$ satisfies the Schrödinger equation for the total Hamiltonian $\hat{H}$, the wave function in the interaction picture satisfies the following equation:

$$i\hbar \frac{\partial}{\partial t} \, |\Phi(t)\rangle \, = \hat{W}_I(t) \, |\Phi(t)\rangle \, .$$

2. The evolution operator in the interaction picture is introduced via the relation

$$|\Phi(t)\rangle \, = \hat{U}_I(t) \, |\Phi(0)\rangle \, .$$

   a. Prove that the evolution operator satisfies the equation

$$i\hbar \frac{\partial}{\partial t} \hat{U}_I(t) = \hat{W}_I(t) \hat{U}_I(t).$$

$\Big[$ *Hint:* Keep in mind that $|\Phi(0)\rangle = |\Psi(0)\rangle$, as immediately follows from the definition of $|\Phi(t)\rangle$. $\Big]$

b. Show that if $|\Phi(t)\rangle = \hat{U}_I(t)\,|\Phi(0)\rangle$, then

$$\begin{aligned} |\Psi(t)\rangle =& \hat{U}(t)\,|\Psi(0)\rangle\ , \text{ where} \\ \hat{U}(t) =& e^{-\frac{i}{\hbar}\hat{H}_0 t}\hat{U}_I(t). \end{aligned}$$

3. Show how the differential equation for the evolution operator can be transformed to an integral equation

$$\hat{U}_I(t) = \hat{I} - \frac{i}{\hbar}\int_0^t dt_1 \hat{W}_I(t_1)\hat{U}_I(t_1).$$

II. SPIN AND ORBITAL MOMENTS

A. Kramers doublet

The action of the angular momentum opeartor, $\hat{\mathbf{L}}$, on a state $|m,l\rangle$ characterized by well-defined values of the angular momentum l and its projection m, is defined by the following formulae:

$$\begin{aligned} \hat{L}_x\,|m,l\rangle =& \sqrt{(l+m+1)(l-m)}\,|m+1,l\rangle + \sqrt{(l+m)(l-m+1)}\,|m-1,l\rangle\ , \\ \hat{L}_y\,|m,l\rangle =& \frac{1}{i}\left(\sqrt{(l+m+1)(l-m)}\,|m+1,l\rangle - \sqrt{(l+m)(l-m+1)}\,|m-1,l\rangle\right), \\ \hat{L}_z\,|m,l\rangle =& m\,|m,l\rangle\ . \end{aligned}$$

The formulae apply also to a particular case of the spin operator, $\hat{\mathbf{S}}$ (with $l = 1/2$, $m = \pm 1/2$).

Consider a system characterized by an orbital moment $l = 1$ and a spin $s = 1/2$. (Such a system is realized in a low-energy description of many transition-metal compounds.) Let us designate the states of such a system as $|m;\sigma\rangle$, where $m = 0, \pm 1$ is a projection of the orbital momentum and $\sigma =\uparrow,\downarrow$ the spin state. These states are obviously the eignestates of both the orbital momentum $\hat{\mathbf{L}}$ and spin $\hat{\mathbf{S}}$.

Define two new states (so-called *Kramers doublet*)

$$\begin{aligned} \left|\tilde{\uparrow}\right\rangle =& \sin\theta\,|0;\uparrow\rangle - \cos\theta\,|+1;\downarrow\rangle\ , \\ \left|\tilde{\downarrow}\right\rangle =& \sin\theta\,|0;\downarrow\rangle - \cos\theta\,|-1;\uparrow\rangle\ , \end{aligned}$$

where θ is just some angle. (These states are not the eigenstates of $\hat{\mathbf{L}}$ and $\hat{\mathbf{S}}$.)

1. Evaluate the average orbital momentum and spin,

a.

$$\left\langle\tilde{\uparrow}\middle|\hat{L}_x\middle|\tilde{\uparrow}\right\rangle, \qquad \left\langle\tilde{\uparrow}\middle|\hat{L}_y\middle|\tilde{\uparrow}\right\rangle, \qquad \left\langle\tilde{\uparrow}\middle|\hat{L}_z\middle|\tilde{\uparrow}\right\rangle,$$

b.

$$\left\langle\tilde{\uparrow}\middle|\hat{S}_x\middle|\tilde{\uparrow}\right\rangle, \qquad \left\langle\tilde{\uparrow}\middle|\hat{S}_y\middle|\tilde{\uparrow}\right\rangle, \qquad \left\langle\tilde{\uparrow}\middle|\hat{S}_z\middle|\tilde{\uparrow}\right\rangle.$$

2. Evaluate the average values of $\hat{\mathbf{L}}^2$ and $\hat{\mathbf{S}}^2$,

$$\left\langle\tilde{\uparrow}\middle|\hat{\mathbf{L}}^2\middle|\tilde{\uparrow}\right\rangle, \qquad \left\langle\tilde{\uparrow}\middle|\hat{\mathbf{S}}^2\middle|\tilde{\uparrow}\right\rangle,$$

   and show that they are the same as for the original states $|\pm1;\uparrow\rangle$.
   [*Hint:* Use the identities: $\hat{\mathbf{L}}^2 = \hat{L}_-\hat{L}_+ + \hat{L}_z^2 + \hat{L}_z$, $\hat{\mathbf{S}}^2 = \hat{S}_-\hat{S}_+ + \hat{S}_z^2 + \hat{S}_z$.]

B. Fierz identity

1. Prove the Fierz identity,

$$2\delta_{\alpha\mu}\delta_{\nu\beta} = \delta_{\alpha\beta}\delta_{\nu\mu} + \vec{\sigma}_{\alpha\beta}\vec{\sigma}_{\nu\mu},$$

   where $\vec{\sigma}_{\alpha\beta}$ are Pauli matrices.

2. Consider operators $\hat{c}_\alpha$, $\hat{c}_\alpha^\dagger$, $\hat{f}_\alpha$, $\hat{f}_\alpha^\dagger$, depending on spin index α. Prove an identity,

$$(\hat{c}_\alpha^\dagger\hat{f}_\alpha)(\hat{f}_\beta^\dagger\hat{c}_\beta) = \frac{1}{2}\hat{c}_\alpha^\dagger\hat{c}_\alpha\hat{f}_\beta^\dagger\hat{f}_\beta - (\hat{c}_\alpha^\dagger\vec{\sigma}_{\alpha\beta}\hat{c}_\beta)(\hat{f}_\nu^\dagger\vec{\sigma}_{\nu\mu}\hat{f}_\mu)$$

III. (*) SCREENING OF THE NUCLEUS CHARGE

The radial part of the ground-state wave function of a hydrogen-like atom is given by

$$R_{0,0}(r) = \frac{Z^{3/2}}{\sqrt{\pi}}e^{-Zr},$$

where Z is the nucleus charge.

1. Find the radial part of the electron charge density, $\rho(r)$, in the ground state. (Mind the sign of the electron charge.)

2. Consider a case $Z = 1$ and evaluate the potential generated by electrons, $\phi_e(r)$. To do this, use the Poisson equation for spherically symmetric potentials,

$$\frac{1}{r}\frac{d^2}{dr^2}(r\phi_e(r)) = -4\pi\rho(r),$$

   and find the solution which is finite at $r = 0$ and vanishes at infinity.

3. The total potential of the atom is a sum of the electron potential $\phi_e(r)$ and a nucleus contribution $\phi_{\text{nucl}}(r) = Z/r$. Evaluate the total potential for $Z = 1$ and demonstrate explicitly its asymptotical behavior at $r \to \infty$.

4. Consider a model of independent electrons for a neutral atom with $Z \geq 1$ and find the total potential in this general case.