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physics606 – Advanced Quantum Theory

Problem Set 6

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problem number	achieved points	possible points
1	14	14
2	7	7
3	6	15
total		36

1 Transitions between general states

1.1 Equivalence of pictures

1/1

Problem statement

Show that H_0 is the same in the Schrödinger and interaction pictures.

In the interaction picture, the operators are defined as

$$O_\mathrm{I}(t) = U_0^\dagger(t, t_0) O_\mathrm{S}(t) U_0(t, t_0)$$

because the states are defined as

$$|\psi, t\rangle_\mathrm{I} = U_0^\dagger(t, t_0) |\psi, t\rangle_\mathrm{S}.$$

In the short form without functional dependence, we have:

$$H_\mathrm{I} = U_0^\dagger H_{0\mathrm{S}} U_0$$

U_0 and H_0 commute since U_0 is a smooth function of H_0 only. ✓

$$= U_0^\dagger U_0 H_{0\mathrm{S}}$$

Now $U_0 U_0^\dagger = 1$. We have

$$= H_{0S}.$$

So $H_I = H_S$.

1.2 Orthogonality and coefficients

2/2

Problem statement

In order to make contact with the results derived in class, express the states $|\alpha\rangle$ and $|\beta\rangle$ as linear superpositions of eigenstates $|n^{(0)}\rangle$ of H_0.

We call those coefficients c and d:

$$|\alpha\rangle = \sum_i c_i |i^{(0)}\rangle, \quad |\beta\rangle = \sum_i d_i |i^{(0)}\rangle.$$ ✓

Since they are eigenstates to the operator O, which seems to be time independent, the states do not depend on the time, just like the eigenstates of the Hamiltonian do not either.

The overlap between the two states is

$$\begin{aligned}\langle\alpha|\beta\rangle &= \sum_i \sum_j c_i^* d_j \langle i^{(0)}|j^{(0)}\rangle \\ &= \sum_i \sum_j c_i^* d_j \delta_{ij} \\ &= \sum_i c_i^* d_i.\end{aligned}$$

The desired orthogonality of the states $|\alpha\rangle$ and $|\beta\rangle$ requires

$$\sum_i c_i^* d_i = 0$$ √

since the c and d are considered to belong to two different states.

1.3 Schrödinger picture 2/2

Problem statement

Show that the probability that $|\psi, t\rangle_S = |\beta\rangle$ is in general non-zero for $t > t_0$ even if $H_1 = 0$ if $[H_0, O_S] \neq 0$.

The state $|\psi, t\rangle_S$ is not a basis vector in the energy basis (the eigenbasis of H_0). Since $[H_0, O_S] \neq 0$, O_S does not need to be diagonal in the general case. (Only commuting operators have the same eigenfunctions and therefore the same eigenbasis and can be diagonalized by the same basis transformation.) Since $|\psi, t\rangle_S$ is not an eigenvector of H_0, the time evolution—that is generated by H_0—will map this to a different vector, which might have an overlap integral with $|\beta\rangle$.

This can also be seen in the calculation. The probability is given by:

$$|\langle\beta|\psi_S(t)\rangle|^2 = |\langle\beta|U_0(t,t_0)|\alpha\rangle|^2$$

Expand into coefficients.

$$= \left|\sum_i\sum_j d_i^* c_j \langle i^{(0)}|U_0(t,t_0)|j^{(0)}\rangle\right|^2$$

Insert U. It is important to note that $H_0[t-t_0]$ is a product of H_0 and $t-t_0$, not a function evaluation. I use square brackets for grouping of this sort for this exact reason, and only round parentheses for function application.

$$= \left|\sum_i\sum_j d_i^* c_j \left\langle i^{(0)}\right| \exp\left(-\frac{\mathrm{i}}{\hbar}H_0[t-t_0]\right)\left|j^{(0)}\right\rangle\right|^2$$

Apply H to the state $|j^{(0)}\rangle$. If this is unclear, expand the exponential function, apply each summand individually and wrap it up in an exponential again.

$$= \left|\sum_i\sum_j d_i^* c_j \left\langle i^{(0)}\right| \exp\left(-\frac{\mathrm{i}}{\hbar}E_j[t-t_0]\right)\left|j^{(0)}\right\rangle\right|^2$$

We can pull this up front now.

$$\surd = \left|\sum_i\sum_j d_i^* c_j \exp\left(-\frac{\mathrm{i}}{\hbar}E_j[t-t_0]\right)\langle i^{(0)}|j^{(0)}\rangle\right|^2$$

That is a δ_{ij} in the back.

$$\surd = \left|\sum_i d_i^* c_i \exp\left(-\frac{\mathrm{i}}{\hbar}E_i[t-t_0]\right)\right|^2$$

For $t = t_0$, this reproduces the previous equation, and we concluded that this had to be 0 since $\delta_{\alpha\beta} = 0$ for $\alpha \neq \beta$. For $t > t_0$ the exponential will change the summands in a way that they do not cancel out together, giving a finite possibility.

1.4 Interaction picture

Here, the probability is

$$|\langle\beta|\psi_I(t)\rangle|^2 = \left|\sum_i d_i^* \langle i^{(0)}|\psi_I(t)\rangle\right|^2.$$

Since the interaction picture is defined such that the action of U_0 is reversed on the states, the states here are actually time independent now:

$$= \left| \sum_i d_i^* \langle i^{(0)} | \alpha \rangle \right|^2 .$$

We expand again.

$$= \left| \sum_i \sum_j d_i^* c_j \langle i^{(0)} | j^{(0)} \rangle \right|^2$$

Same as in the above problem.

$$\surd = \left| \sum_i d_i^* c_i \right|^2$$

For $\alpha \neq \beta$, this is

$$\surd = 0.$$

That is different than the result of the previous part.

Problem statement

The discrepancy to the result of the previous subsection clearly shows that the wave function, or state vector, by itself has no direct physical meaning, even though one of the axioms of quantum mechanics state that it contains all the information about the system that can be known!

Well, $|\psi, t\rangle_I \neq |\psi, t\rangle_S$. There is a U or $U^\dagger$ of difference, depending on your point of view. Since a unitary transformation can be thought of a basis change, it is not too surprising that the scalar product changes when one of the vectors is transformed only ($|\beta\rangle$ is left unchanged). I'd be worried if it was the same when time evolution is taken into account and disregarded. :)

That's exactly the purpose of this question (I suppose)

1.5 Physical meaning

5/5

The expectation value of an operator in the Schrödinger picture is:

$$\langle O_S \rangle = \langle \psi_S(t) | O_S | \psi_S(t) \rangle$$

We write down the time evolution explicitly.

$$= \langle \alpha | U_S^\dagger(t, t_0) O_S U_S(t, t_0) | \alpha \rangle$$

We insert complete set of eigenstates. We also use Greek letters here to distinguish the eigenstates of O from the eigenstates of H_0.

$$= \sum_\gamma \sum_\eta \langle \alpha | U_S^\dagger(t, t_0) | \gamma \rangle \langle \gamma | O_S | \eta \rangle \langle \eta | U_S(t, t_0) | \alpha \rangle$$

The middle part gives us $o_\eta \delta_{\gamma\eta}$.

$$= \sum_\gamma o_\gamma \langle \alpha | U_S^\dagger(t, t_0) | \gamma \rangle \langle \gamma | U_S(t, t_0) | \alpha \rangle$$

We prepare ...

$$= \sum_\gamma o_\gamma \langle \gamma | U_S(t, t_0) | \alpha \rangle^* \langle \gamma | U_S(t, t_0) | \alpha \rangle$$

... and write this as the modulus squared

$$= \sum_\gamma o_\gamma |\langle \gamma | U_S(t, t_0) | \alpha \rangle|^2$$

This could also be written as the probability that the system will go to the state $|\gamma\rangle$ on the measurement.

$$= \sum_\gamma o_\gamma |\langle \gamma | \psi_S(t) \rangle|^2$$

That is more or less one of the axioms of quantum mechanics, that the measurement will turn out to be an eigenvalue of the operator (here o_γ) and that the probabilities are the overlap integrals modulus squared.

Now we can re-complexify the probability part to match the version on the problem set.

$$P_{\beta\alpha} = |\langle \beta | U_S(t, t_0) | \alpha \rangle|^2$$

We insert another set of eigenstates, now the eigenstates of H_0.

$$= \left| \sum_i \sum_f \langle \beta | f^{(0)} \rangle \langle f^{(0)} | U_S(t, t_0) | i^{(0)} \rangle \langle i^{(0)} | \alpha \rangle \right|^2$$

We rearrange those scalar product, they are just scalars and commute.

$$= \left| \sum_i \sum_f \langle i^{(0)} | \alpha \rangle \langle \beta | f^{(0)} \rangle \langle f^{(0)} | U_S(t, t_0) | i^{(0)} \rangle \right|^2$$

Using the given name for the matrix element, we can write this as

$$= \left| \sum_i \sum_f \langle i^{(0)} | \alpha \rangle \langle \beta | f^{(0)} \rangle \mathscr{A}_{fi}(t, t_0) \right|^2 .$$

1.6 Same result

2/2

Physical reality should not change with a (passive) basis transformation. If that would be the case, the different pictures would not be legitimate and not taught at university. (Occam's razor.)

Mathematically, the expectation value is a scalar product where an operator is pre- and postmultiplied by the same wavefunction. Unitary transformations of all kinds cannot change this scalar product, since the basis of everything is changed consistently such that the scalar product does not change. Hence the definition of the operators the way we wrote in the very first part of this problem.

2 Selection rules

2.1 Forbidden transitions 2/2

$[H_1, O] = 0$ means that both operators have the same set of eigenfunctions. Since the state on the right has eigenvalue o_i of the operator O, they are eigenfunctions of O. Therefore, they are also eigenfunctions to H_1. H_1 cannot change the o_i therefore, since it is diagonal in this eigenbasis of O. So $\langle o_f | H_1 | o_i \rangle = \lambda \langle o_f | o_i \rangle = 0$, where λ is the unknown eigenvalue of H_1 to $|o_i\rangle$.

2.2 All orders of perturbation theory 2/2

"All orders" sounds like the Dyson series. There, the perturbation is exponentiated. Since the perturbation itself is diagonal in the space spanned by the eigenstates of O, there is no way (infinitely) repeated application could get it off-diagonal. I do not see how our argument is limited to first order. It's not.

2.3 Angular momentum 3/3

Side question

Is that really $[H_0, \boldsymbol{L}] = 0$? If so, it should be the null vector, like $[H_0, \boldsymbol{L}] = \mathbf{0}$ in the first place. Then, this would imply that all the components of the angular momentum can be measured at the same time with arbitrary precision. This would only work if there is no potential. To us, $[H_0, L^2] = 0$ looks more familiar. Is it really $[H_0, L]$?

No it's L^2 ..

If it was $[H_0, \boldsymbol{L}^2] = 0$, then the eigenstates would be $|n, l, m_l\rangle$. With a perturbation $H_1 = f(z, t)$ the commutator $[H_1, L_3]$ would be zero, forcing m_l to stay unchanged in transitions. The second perturbation depends only on the radius and would l and m_l unchanged.

3 Atomic radiative transitions

3.1 Expansion

We chose the coordinate system such that $\epsilon \parallel \hat{e}_3$. Then the scalar product is

$$\epsilon \boldsymbol{x}_e = \epsilon_3 x_{e,3}.$$

Then we can use spherical coordinates:

$$= \epsilon_3 r_e \cos(\theta_e).$$

Since $Y_{1,0}(\theta, \phi) \propto \cos(\theta)$ and the ϕ part is arbitrary, we can write this as

$$= r_e c_0(\epsilon) Y_{1,0}(\theta_e, \phi_e)$$

where we moved the ϵ_3 component into the coefficient. From there, one can just add more terms to it, the coefficients just have to match.

$$= r_e \sum_m c_m(\epsilon) Y_{1,m}(\theta_e, \phi_e)$$

3.2 Magnetic moment

3.3 Absorption

3.4 Second order

3.5 Rydberg states 3/3

Since n and l is large, and likely transitions only decrease l by one, it will take many transitions. Also, $l \leq n$ has to hold, so n cannot decrease arbitrarily, just along with n. Then the energy differences between states is given by

$$\Delta E = E_{\text{Ryd}} \left[\frac{1}{m^2} - \frac{1}{n^2} \right]. \quad \surd$$

Since m and n are both large in the involved transitions, ΔE will be small. Then

$$\Delta E = \hbar\omega \iff \omega = \frac{\Delta E}{\hbar}$$

such that the frequency is small as well. The transition rate goes with ω^3, which is even smaller than small. $\surd$

The combination of a large number of transitions and the unlikeliness together make for a long lifetime. $\surd$