Physics 501-22

Unitary, Interaction Rep

As mentioned in the last note, we can solve the Shroedinger equation formally by defining the Unitary matrix, $U(t,t')$

$$i\frac{d}{dt}U(t,t') = H(t)U(t,t') \tag{1}$$

where multiplication is matrix (or operator) multiplication. The formal solution to this is

$$U(t,t') = \mathbf{T}e^{-i\int_{t'}^{t} H(t_1)}dt_1 \tag{2}$$

where $\mathbf{T}$ is the time ordering operator. Ie, expand the exponential into its taylor series, and in each of the terms rearrange all the $H(t_1)$ so that the later time operators are all to the left of any earlier time operators. This ensures that $U(t,t') = U(t,\tilde{t})U(\tilde{t},t')$ which we would want for the operators, but would not be true if the $\mathbf{T}$ were not there. Ie,

$$\begin{aligned} U(t,t') &= \lim_{N\to\infty} U(t'+N\tau, t'+(N-1)\tau)U(t'+(N-1)\tau, t'-(N-2)\tau) && (3)\\ &\quad ...U(t'+2\tau, t'+\tau)U(t'+\tau, t') && (4)\end{aligned}$$

where $\tau = \frac{t-t'}{N}$.

As stated, in Schoedinger representation,

$$|\psi\rangle(t) = U(t,t')|\psi\rangle(t') \tag{5}$$

In the Heisenberg representation, H is the Hamiltonian in terms of the time dependent dynamic variables, H(P(t),X(t),t). The equation of motion for a dynamic variable is

$$i\frac{d}{dt}A(P(t),X(t)) = [A(P(t),X(t)), H(P(t),X(t),t)] \tag{6}$$

Defining

$$i\frac{d}{dt}U_H(t,t') = H(P(t),X(t),t)U_H(t,t') \tag{7}$$

$$U(t',t') = I \tag{8}$$

where I is the identity operator, and defining

$$\begin{aligned} A(t) &= U^\dagger(t,t')A(P(t'),X(t'))U(t,t') && (9)\\ &= A(U^\dagger(t,t')P(t')U(t,t'), U^\dagger(t,t')X(t')U(t,t')) = A(P(t),X(t)) && (10)\end{aligned}$$

Then

$$\begin{aligned} i\frac{dA(t)}{dt} &= -U^\dagger(t,t')H(t,P(0),X(0))A(t')U(t,t') + U^\dagger(t,t')A(t')H(t,P(t'),X(t'))U(t,t') && (11)\\ &= -H(t,P(t),X(t))U^\dagger(t,t')A(t')U(t,t') + U^\dagger(t,t')A(t')U(t,t')H(t,P(t),X(t)) && (12)\end{aligned}$$

since $H(t)^\dagger = H(t)$

Note that we can look at the expectation value of the operator A, which, by Born's rule (generalised to a generic operator A ratehr than just X). Let us desinate the expectation value of A by $< A >$

$$< A >= \langle\psi| A |\psi\rangle \tag{13}$$

In the Schroedinger representation, we have

$$< A(t) >= \langle\psi| (t)A |\psi\rangle (t) = (\langle\psi| (t')U^\dagger(t,t'))A(t')(U(t,t') |\psi\rangle (t')) \tag{14}$$

But we can rewrite this as

$$< A(t) >= \langle\psi| (t')(U^\dagger(t,t'))A(t')U(t,t')) |\psi\rangle (t') \tag{15}$$

Intraction Representation

Let us consider a Hamiltonian which is made up of two terms

$$H = H_0 + H_I \tag{16}$$

Define $U,\ U_0$ by

$$i\partial_t U(t,t') = (H_0 + H_I)U(t,t') \tag{17}$$

$$i\partial_t U_0(t,t') = H_0 U_0(t,t') \tag{18}$$

Then we have

$$\begin{aligned} < A(t) > &= \langle\psi| (t')U^\dagger(t,t')A(t')U(t,t') |\psi\rangle (t') = \langle\psi| (t')U^\dagger(t,t')A(t') |\psi\rangle (t') \\ &= (\langle\psi| (t')U^\dagger U_0(t,t'))U_0^\dagger(t,t')A(t')U_0(t,t')(U_0^\dagger U(t,t')) |\psi\rangle (t') \end{aligned} \tag{19}$$

The central term $U_0^\dagger(t,t')A(t')U_0(t,t')$ is just the Heisenberg evolution of A if the Hamiltonian were H_0. The state $(U_0^\dagger U(t,t')) |\psi\rangle (t')$ is the Schrodinger representation state as though the evolution were driven by the Unitary operator $(U_0^\dagger U(t,t'))$. This obeys the equation

$$i\frac{d}{dt}(U_0^\dagger(t,t')U(t,t')) \tag{20}$$

$$\begin{aligned} &= -U_0^\dagger(t,t')H_0U(t,t') + U_0(t,t')(H_0 + H_I)U(t,t') \\ &= U_0^\dagger(t,t')H_IU_0(t,t')U_0^\dagger(t,t')U(t,t') \end{aligned} \tag{21}$$

but $U_0^\dagger(t,t')H_IU_0(t,t')$ is the Heisenberg evolution operator for the operator H_I. In general, even if H_0 and H_I are not explicitly time dependent, $U_0^\dagger(t,t')H_IU_0(t,t')$ will be time dependent since

$$U_0^\dagger(t,t')H_I(P,X)U_0(t,t') \tag{22}$$

$$\begin{aligned} &= H_I(U_0^\dagger(t,t'))P(t')U_0(t,t'), U_0^\dagger(t,t')X(t')U_0(t,t')) \\ &= H_I(P(t),X(t)) \end{aligned} \tag{23}$$

is in general explicitly time dependent.

If it is the case that the Hamiltonian H_0 were easily solveable in the Heisenberg representation, then one could simplify the solution by first solving the Heisenberg equation, substituting them in H_I and then solve the Schroedinger representation for the state in the interaction representation. If H_I is small (eg, is multiplied by a small coupling constant) then one could solve that new Schroedinger equation perturbatively. The Heisenberg state for $P(t), X(t)$ should stay near the intial state.

One can solve the system perturbatively, either with the Magnus expansion of the unitary operator, since each successive Ω_n will have an exptra small parameter ϵ, or with the Dyson expansion, in which one writes $|\psi_I\rangle$ as a power series in ϵ, and solves the equation power by power in ϵ.

Lets take an example

$$H = \frac{1}{2}(P^2 + X^2) + \epsilon(t)X \tag{24}$$

with $H_0 = \frac{1}{2}(P^2 + X^2)$. This is of course easily solveable if ϵ is constant. Defining $Y = X + epsilon$, then P is the conjugate momentum for Y as well, and the Hamiltonian becomes $H = \frac{1}{2}(P^2 + Y^2 - \epsilon^2)$ which we know how to solve in either the Heisenberg or Schroedinger representations for all values of ϵ, but that is not the point here and is not easily solvable if ϵ is a function of time. Let us look at that solution in the Interaction representation with epsilon constant.

The Heisenberg equations for H_0 are

$$\partial_t X = -i[X, H_0] = P \tag{25}$$

$$\partial_t P = -i[P, X] = -X \tag{26}$$

Taking $t' = 0$, the solution is

$$P_0(t) = P(0)cos(t) - X(0)sin(t) \tag{27}$$

$$X_0(t) = X(0)cos(t) + P(0)sin(t) \tag{28}$$

then we have the interaction representation perturbation operator

$$H_I = \epsilon(X(0)cos(t) + P(0)sin(t)) \tag{29}$$

This is clearly time dependent.

Let us assume that we start with the ground state of the H_0 for the the intial state. In the X basis this would be $\psi_0(x) = \frac{e^{-x^2/2}}{(2\pi)^{1/4}}$. Then the equation for $\psi(x,t)$ would be

$$i\frac{d}{dt}\psi(x,t) = \epsilon(x\cos(t) - i\sin(t)\partial_x)\psi(x,t) \tag{30}$$

In the Dyson expansion we would write

$$\psi(x,t) = \sum_n \epsilon^n \psi_n(x,t) \tag{31}$$

and equating the equation power by power of ϵ

$$\dot{\psi}_n(t,x) = (x\cos(t) - i\sin(t)\partial_x)\psi_{n-1}(t,x) \tag{32}$$

Thus

$$\begin{aligned} i\dot{\psi}_1 &= (x\cos(t) - i\sin(t)\partial_x)\psi_0(x) && (33)\\ i\dot{\psi}_2 &= (x\cos(t) - i\sin(t)\partial_x)\psi_0(x) && (34)\\ \dots & && (35) \end{aligned}$$

The first equation becomes (recalling that $P = -i\partial_x$

$$\psi_1 = -i\int(e^{-x^2/2}(cos(t)x + isin(t)x)\psi_0(x)dt = -xe^{-x^2}(e^{it} - 1) \tag{36}$$

The second becomes

$$\begin{aligned} \psi_2 &= e^{-x^2/2}\left(e^{2*I*t}(\frac{-2x^2+1)}{4}) + e^{it}(\frac{-2x^2+1}{2}\right. && (37)\\ &\left. +\frac{1}{2}x^2 - \frac{3}{4} + \frac{1}{2}it + \frac{1}{2}e^{-it}\right) && (38) \end{aligned}$$

and one can continue in this way with successive terms becoming more and more complex. Furthermore, if we truncate at some order N, then $\sum_0^N \epsilon^n\psi_n$ will not have unit norm, even if ψ_0 is. The transformation is not unitary.

The Magnus exansion is simplified because

$$[H_I(t), H_I(t'')] = i\epsilon^2(\cos(t)\sin(t'') - \sin(t)\cos(t'')) \tag{39}$$

is a c-number and thus all of the higher order terms than Ω_2 in the expansion are zero since they contain the commutator of a C number with an operator, which is 0. Thus

$$\begin{aligned} \Omega &= \epsilon(sin(t)x - i(cos(t) - 1)\partial_x) && (40)\\ &-i\epsilon^2\int_0^t\int_0^{t_1}(\frac{1}{2}(\cos(t_1)\sin(t_2) - \sin(t_1)\cos(t_2))dt_2dt_1 && (41) \end{aligned}$$

The second term is just a phase, and can be ignored. Now, by the BakerCambellHausorff relation, if the commutator of A and B is a C number, then

$$e^{A/2}e^Be^{A/2} = e^{A+B} \tag{42}$$

Thus

$$e^{\alpha X+\beta P} = e^{\alpha X/2}e^{\beta P}e^{\alpha X/2} \tag{43}$$

Now,

$$e^{\beta P}f(x) = \sum_n\frac{\beta^n(-i\partial_x)^n}{n!}f(x) = \sum_n\frac{(-i\beta)^n}{n!}\partial_x^nf(x) = f(x - i\beta) \tag{44}$$

where the last terms comes from the Taylor series expansion of f.

Thus

$$e^{\epsilon(sin(t)X+(cos(t)-1)P)}f(x) = e^{sin(t)x/2}e^{(cos(t)-1)P}(e^{x\sin(t)/2}e^{-x^2/2} \tag{45}$$

$$= e^{sin(t)x/2+(x-i(cos(t)-1))sin(t)/2-(x-i(cos(t)-1))^2/2} \tag{46}$$

Thus the Magnus expansion gives the exact solution in the interaction representation.

Even if ϵ is a function of t, this allow us to solve the equation exactly. That only the first two terms in the Magnus expansion are non-zero is still true, and that the second term is an imaginary C-number since the exponential of this term must be unitary, and the only unitary C-number is a pure phase, is also still true.

Of course, in general it is not that simple. The Magnus expansion does not usually terminate, and the first exponential is in general not easy to evaluate. Thus it is usually the Dyson expansion that is used in the interaction picture.