Recapitulación

Operadores unitarios $\hat{U}^\dagger \hat{U} = \hat{U}\hat{U}^\dagger = \mathbb{1}$

$|\tilde{\psi}\rangle = U|\psi\rangle$

Preserva producto punto $\langle\tilde{\psi}|\tilde{\varphi}\rangle = \langle\psi|\varphi\rangle$

$\hat{U}$ unitario $\iff$ $\hat{U}$ transforma base ortonormal en base ortonormal.

Def de operador transformado

$\langle\tilde{b}_i|\tilde{A}|\tilde{b}_j\rangle = \langle b_i|A|b_j\rangle \Rightarrow U^\dagger \tilde{A} U = A$

$\tilde{A} = UAU^\dagger$

$\widetilde{F(A)} = F(\tilde{A})$

- Transformaciones de operadores: Si tenemos A un operador y $\{|v_i\rangle\}$ una base ortonormal. Definimos $\tilde{A}$ como el operador que en la base $\{|\tilde{v}_i\rangle\}$ obtenida de aplicar U a $\{|v_i\rangle\}$ tiene los mismos elementos de matriz que el operador A en la base $\{|v_i\rangle\}$.

$$\text{Def} \qquad \langle\tilde{v}_i|\tilde{A}|\tilde{v}_j\rangle = \langle v_i|A|v_j\rangle$$

$$\langle v_i|U^\dagger A U|v_j\rangle$$

entonces $U^\dagger \tilde{A} U = A$ o bien $\tilde{A} = UAU^\dagger$.

- Como

$$\left(\tilde{A}\right)^2 = UAU^\dagger UAU^\dagger = UA^2U^\dagger = \widetilde{A^2}$$

podemos generalizar esto para ver que $\widetilde{F(A)} = F(\tilde{A})$.

- Si los eigenvectores de A son $|\phi_n\rangle$ los de $\tilde{A}$ son $\left|\tilde{\phi}_n\right\rangle$. Los eigenvalores son los mismos.

Veamos ↓

How can the eigenvectors of $\tilde{A}$ be obtained from those of A? Let us consider an eigenvector $|\varphi_a\rangle$ of A, with an eigenvalue a:

$$A|\varphi_a\rangle = a|\varphi_a\rangle \tag{31}$$

Let $|\tilde{\varphi}_a\rangle$ be the transform of $|\varphi_a\rangle$ by the operator U: $|\tilde{\varphi}_a\rangle = U|\varphi_a\rangle$. We then have:

$$\begin{aligned}\tilde{A}|\tilde{\varphi}_a\rangle &= (UAU^\dagger)U|\varphi_a\rangle = UA(U^\dagger U)|\varphi_a\rangle \\ &= UA|\varphi_a\rangle = aU|\varphi_a\rangle \\ &= a|\tilde{\varphi}_a\rangle\end{aligned} \tag{32}$$

Ejemplo: operador de evolución

Como la transformación $|\psi(t_0)\rangle \longrightarrow |\psi(t)\rangle$ es lineal
$\exists$ un operador de evolución

$$|\psi(t)\rangle = U(t,t_0)\,|\psi(t_0)\rangle \qquad U(t,t) = \mathbb{1}$$

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H\,|\psi(t)\rangle$$

$$i\hbar\frac{\partial}{\partial t}U\,|\psi(t_0)\rangle = HU\,|\psi(t_0)\rangle$$ porque $|\psi(t_0)\rangle$ es arbitrario

$$i\hbar\frac{\partial}{\partial t}U = HU$$

Con la condición inicial $U(t_0,t_0) = \mathbb{1}$, $i\hbar\frac{\partial}{\partial t}U = HU$ define U.

Para un sistema conservativo

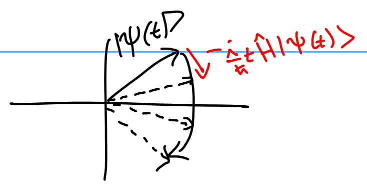
$$U(t,t_0) = e^{-iH(t-t_0)/\hbar}$$

Es unitario pues es $e^{i\,\text{Hermitiano}}$

pero para justificarlo bien debemos aprender a derivar operadores respecto a un parámetro real.

U nos ayuda a interpretar el significado de aplicar H. $\quad |\psi'\rangle = H|\psi\rangle$

Para tiempos cortos $(t_0=0)$ $\quad \hat{U}(\Delta t) \approx \mathbb{1} + \frac{1}{i\hbar}\hat{H}\Delta t + \cdots$



si $i\hbar\frac{d}{dt}|\psi\rangle = H|\psi\rangle \;\rightsquigarrow\; \frac{|\psi(t+\Delta t)\rangle - |\psi(t)\rangle}{\Delta t} = \frac{1}{i\hbar}H|\psi\rangle$

$\rightsquigarrow |\psi(t+\Delta t)\rangle = |\psi(t)\rangle + \frac{\Delta t}{i\hbar}H|\psi(t)\rangle$

Para $A(t)$ definimos $\frac{\mathrm{d}A}{\mathrm{d}t} = \lim_{\Delta t \to 0} \frac{A(t+\Delta t) - A(t)}{\Delta t}$

Como $\langle u_i | A(t) | u_j \rangle = A_{ij}(t)$

Let us call $\left(\frac{\mathrm{d}A}{\mathrm{d}t}\right)_{ij} = \left\langle u_i \middle| \frac{\mathrm{d}A}{\mathrm{d}t} \middle| u_j \right\rangle$ the matrix elements of $\frac{\mathrm{d}A}{\mathrm{d}t}$. It is easy to verify the relation:

$$\left(\frac{\mathrm{d}A}{\mathrm{d}t}\right)_{ij} = \frac{\mathrm{d}}{\mathrm{d}t} A_{ij} \tag{54}$$

$$\left(\frac{dA}{dt}\right)_{ij} = \langle u_i | \lim_{\Delta t \to 0} \frac{A(t+\Delta t) - A(t)}{\Delta t} | u_j \rangle = \lim_{\Delta t \to 0} \frac{A_{ij}(t+\Delta t) - A_{ij}(t)}{\Delta t} = \frac{d}{dt} A_{ij}(t)$$

lim lineal

5-b. Differentiation rules

They are analogous to the ones for ordinary functions:

$$\frac{\mathrm{d}}{\mathrm{d}t}(F+G) = \frac{\mathrm{d}F}{\mathrm{d}t} + \frac{\mathrm{d}G}{\mathrm{d}t} \tag{55}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(FG) = \frac{\mathrm{d}F}{\mathrm{d}t} G + F \frac{\mathrm{d}G}{\mathrm{d}t} \tag{56}$$

Nevertheless, care must be taken not to modify the order of the operators in formula (56).

Let us prove, for example, the second of these equations. The matrix elements of FG are:

$$\langle u_i | FG | u_j \rangle = \sum_k \langle u_i | F | u_k \rangle \langle u_k | G | u_j \rangle \tag{57}$$

We have seen that the matrix elements of $\mathrm{d}(FG)/\mathrm{d}t$ are the derivatives with respect to t of those of (FG). Thus we have, taking the derivative of the right-hand side of (57):

$$\left\langle u_i \middle| \frac{\mathrm{d}}{\mathrm{d}t}(FG) \middle| u_j \right\rangle = \sum_k \left[\left\langle u_i \middle| \frac{\mathrm{d}F}{\mathrm{d}t} \middle| u_k \right\rangle \langle u_k | G | u_j \rangle + \langle u_i | F | u_k \rangle \left\langle u_k \middle| \frac{\mathrm{d}G}{\mathrm{d}t} \middle| u_j \right\rangle \right]$$
$$= \left\langle u_i \middle| \frac{\mathrm{d}F}{\mathrm{d}t} G + F \frac{\mathrm{d}G}{\mathrm{d}t} \middle| u_j \right\rangle \tag{58}$$

más claro

This equation is valid for any i and j. Formula (56) is thus established.

$$\langle u_i | \frac{d}{dt}(FG) | u_j \rangle = \frac{d}{dt} \langle u_i | FG | u_j \rangle$$

$$= \frac{d}{dt} \sum_k \langle u_i | F | u_k \rangle \langle u_k | G | u_j \rangle$$

escalares

$$= \sum_k \left(\frac{d}{dt} \langle u_i | F | u_k \rangle \right) \langle u_k | G | u_j \rangle + \langle u_i | F | u_k \rangle \frac{d}{dt} \langle u_k | G | u_j \rangle$$

$$= \sum_k \langle u_i | \frac{dF}{dt} | u_k \rangle \langle u_k | G | u_j \rangle + \langle u_i | F | u_k \rangle \langle u_k | \frac{dG}{dt} | u_j \rangle$$

$$= \langle u_i | \frac{dF}{dt} G + F \frac{dG}{dt} | u_j \rangle$$

$$\langle u_i | \frac{dA^n}{dt} | u_j \rangle = \frac{d}{dt} \langle u_i | A^n | u_j \rangle$$

$$\langle v_i | \frac{d(t^n M)}{dt} | v_j \rangle = \frac{d}{dt} \langle v_i | t^n M | v_j \rangle$$

$$= \langle v_i | M | v_j \rangle \frac{d}{dt} t^n = n t^{n-1} M_{ij}$$

5-c. Examples

Let us calculate the derivative of the operator e^{At}. By definition, we have:

$$\mathrm{e}^{At} = \sum_{n=0}^{\infty} \frac{(At)^n}{n!}$$

Taking the derivative of the series term by term, we obtain:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{At} &= \sum_{n=0}^{\infty} n \frac{t^{n-1}A^n}{n!} \\
&= A \sum_{n=1}^{\infty} \frac{(At)^{n-1}}{(n-1)!} \\
&= \left[\sum_{n=1}^{\infty} \frac{(At)^{n-1}}{(n-1)!} \right] A
\end{aligned} \tag{60}$$

We recognize inside the brackets the series that defines e^{At} (taking as the summation index $p = n - 1$). The result is therefore:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{At} = A\,\mathrm{e}^{At} = \mathrm{e}^{At} A \tag{61}$$

In this simple case involving only one operator, it is unnecessary to pay attention to the order of the factors: e^{At} and A commute.

This is not the case if one is interested in taking the derivative of an operator such as $\mathrm{e}^{At}\mathrm{e}^{Bt}$. Applying (56) and (61), we obtain:

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathrm{e}^{At}\mathrm{e}^{Bt}) = A\mathrm{e}^{At}\mathrm{e}^{Bt} + \mathrm{e}^{At}\,B\mathrm{e}^{Bt} \tag{62}$$

The right-hand side of this equation can be transformed into $\mathrm{e}^{At}\,A\mathrm{e}^{Bt} + \mathrm{e}^{At}\,B\mathrm{e}^{Bt}$ or $\mathrm{e}^{At}\,A\mathrm{e}^{Bt} + \mathrm{e}^{At}\,\mathrm{e}^{Bt}B$, for example. However, we can never obtain (unless, of course, A and B commute) an expression such as $(A+B)\mathrm{e}^{At}\mathrm{e}^{Bt}$. In this case, the order of the operators is therefore important.

Comment:

Even when the function involves only one operator, taking the derivative cannot always be performed according to the rules valid for ordinary functions. For example, when $A(t)$ has an arbitrary time-dependence, the derivative $\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{A(t)}$ *is generally not equal to* $\frac{\mathrm{d}A}{\mathrm{d}t}\mathrm{e}^{A(t)}$. It can be seen by expanding $\mathrm{e}^{A(t)}$ in a power series in $A(t)$ that $A(t)$ and $\frac{\mathrm{d}A}{\mathrm{d}t}$ must commute for the equality to hold.

Con esto

$$U(t,t_0) = e^{-\frac{i}{\hbar}(t-t_0)H}$$

$$\frac{d}{dt} U = -\frac{i}{\hbar} H e^{-\frac{i}{\hbar}(t-t_0)H} = \frac{1}{i\hbar} HU$$