

La clase pasada vimos:

- Pictures o representaciones: repaso de Schrödinger y Heisenberg
- Picture de interacción o de Dirac
- Ecuación de Tomonaga-Schwinger
- Serie de Dyson

En esta clase veremos:

- Probabilidad de transición
- Tratamiento perturbativo dependiente del tiempo
- Perturbación constante
- Regla de oro de Fermi

Cambio de representación:

$$\begin{aligned}
 |\psi(t)\rangle_A &\equiv A(t)|\psi\rangle \\
 O(t)_A &\equiv A(t)OA^\dagger(t)
 \end{aligned}
 \longrightarrow
 \langle\psi|O|\phi\rangle = \langle\psi_A|O_A|\phi_A\rangle$$

Representación de interacción

Supongamos:

$$H_S = H_0 + V_S$$

$$H_0 \neq H_0(t)$$

$$A(t) \equiv e^{\frac{i}{\hbar}H_0t} \longrightarrow \begin{cases} |\Psi(t)\rangle_I = e^{\frac{i}{\hbar}H_0t} |\Psi(t)\rangle_S \\ O(t)_I = e^{\frac{i}{\hbar}H_0t} O(t)_S e^{-\frac{i}{\hbar}H_0t} \end{cases}$$

En el picture de interacción **evolucionan** los **estados** y los **operadores**

$$i\hbar \frac{d}{dt} O(t)_I = [O(t)_I, H_0] + i\hbar \left[\frac{\partial O}{\partial t} \right]_I$$

$$\left[\frac{\partial O}{\partial t} \right]_I \equiv e^{\frac{i}{\hbar} H_0 t} \left[\frac{\partial O_S}{\partial t} \right] e^{-\frac{i}{\hbar} H_0 t},$$

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle_I = V(t)_I |\Psi(t)\rangle_I$$

Ecuación de Tomonaga-Schwinger

Serie de Dyson

$$U_I(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^t V_I(t') \left[1 - \frac{i}{\hbar} \int_{t_0}^{t'} V_I(t'') U_I(t'', t_0) dt'' \right] dt'$$

exacto

$$= 1 - \frac{i}{\hbar} \int_{t_0}^t dt' V_I(t') + \left(\frac{-i}{\hbar} \right)^2 \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' V_I(t') V_I(t'')$$

órdenes 0, 1 y 2

$$+ \dots + \left(\frac{-i}{\hbar} \right)^n \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' \dots \int_{t_0}^{t^{(n-1)}} dt^{(n)} V_I(t') V_I(t'') \dots V_I(t^{(n)})$$

3 hasta n

+ ...

órdenes mayores que n

Probabilidad de transición

Evolución del estado

Expandamos el estado en representación de interacción en la base de autoestados de H_0 en la rep. de Schrödinger:

$$|\psi(t)\rangle_I = \sum_n c_n(t) |n\rangle \quad \text{Hallar } c_n(t)$$

La evolución del estado está dada por la ecuación de Tomonaga-Schwinger:

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle_I = V_I(t) |\psi(t)\rangle_I = \sum_m V_I(t) |m\rangle \langle m | \psi(t)\rangle_I$$


$$i\hbar \frac{\partial}{\partial t} \overbrace{\langle n | \psi(t)\rangle_I}^{\dot{c}_n(t)} = \sum_m \langle n | V_I(t) | m \rangle \overbrace{\langle m | \psi(t)\rangle_I}^{c_m(t)}$$

$$|\psi(t)\rangle_I = \sum_n c_n(t) |n\rangle \quad \longrightarrow \quad \text{hallar } c_n(t)$$

$$\longrightarrow \quad i\hbar \dot{c}_n(t) = \sum_m \langle n | V_I(t) | m \rangle c_m(t)$$

Notar que: $\langle n | V_I(t) | m \rangle = \langle n | e^{iH_0 t/\hbar} V_S(t) e^{-iH_0 t/\hbar} | m \rangle$

$$\omega_{nm} \equiv \frac{E_n - E_m}{\hbar}$$

$$= e^{i(E_n - E_m)t/\hbar} \langle n | V_S(t) | m \rangle = V_{nm}(t) e^{i\omega_{nm}t}$$

$$\longrightarrow \quad i\hbar \dot{c}_n(t) = \sum_m V_{nm}(t) e^{i\omega_{nm}t} c_m(t)$$



$$i\hbar \dot{c}_n(t) = \sum_m V_{nm}(t) e^{i\omega_{nm}t} c_m(t)$$

(5.5.17)

$$i\hbar \begin{pmatrix} \dot{c}_1 \\ \dot{c}_2 \\ \dot{c}_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} V_{11} & V_{12}e^{i\omega_{12}t} & \cdots \\ V_{21}e^{i\omega_{21}t} & V_{22} & \cdots \\ & & V_{33} & \cdots \\ \vdots & \vdots & & \ddots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix}$$

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Approach perturbativo dependiente del tiempo:

$$i\hbar \begin{pmatrix} \dot{c}_1 \\ \dot{c}_2 \\ \dot{c}_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} V_{11} & V_{12}e^{i\omega_{12}t} & \cdots \\ V_{21}e^{i\omega_{21}t} & V_{22} & \cdots \\ & & V_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix} \quad (5.5.17)$$

equation for $c_n(t)$ are usually not available. We must be content with approximate solutions to (5.5.17) obtained by perturbation expansion:

$$c_n(t) = c_n^{(0)} + c_n^{(1)} + c_n^{(2)} + \cdots, \quad (5.6.1)$$

where $c_n^{(1)}, c_n^{(2)}, \dots$ signify amplitudes of first order, second order, and so on in the strength parameter of the time-dependent potential.

If initially only the state i is populated, we approximate c_n on the right-hand side of differential equation (5.5.17) by $c_n^{(0)} = \delta_{ni}$ (independent of t) and relate it to the time derivative of $c_n^{(1)}$, integrate the differential equation to obtain $c_n^{(1)}$, plug $c_n^{(1)}$ into the right-hand side [of (5.5.17)] again to obtain the differential equation for $c_n^{(2)}$, and so on. This is how Dirac developed time-dependent perturbation theory in 1927.

Tratamiento perturbativo dependiente del tiempo

Supongamos: $|\psi(t_0)\rangle_I = |i\rangle$ donde $H_0|i\rangle = E_i|i\rangle$

$$|\psi(t)\rangle_I = U_I(t, t_0)|\psi(t_0)\rangle_I = U_I(t, t_0)|i\rangle$$

$$\begin{array}{c} \text{➔} \\ \underbrace{\langle n|\psi(t)\rangle_I}_{c_n(t)} = \langle n|U_I(t, t_0)|i\rangle \end{array}$$

Usamos la expansión perturbativa de $U_I(t, t_0)$:

$$c_n^{(0)}(t) = \langle n|1|i\rangle = \delta_{ni}$$

$$c_n(t) = \langle n | \psi(t) \rangle_I = \langle n | U_I(t, t_0) | i \rangle$$

Usamos la expansión perturbativa de $U_I(t, t_0)$:

$$c_n^{(0)}(t) = \langle n | 1 | i \rangle = \delta_{ni}$$

$$c_n^{(1)}(t) = \langle n | \left(\frac{-i}{\hbar} \right) \int_{t_0}^t dt' V_I(t') | i \rangle$$

$$= \left(\frac{-i}{\hbar} \right) \int_{t_0}^t dt' \langle n | e^{iH_0(t'-t_0)/\hbar} V(t') e^{-iH_0(t'-t_0)/\hbar} | i \rangle$$

$$= \left(\frac{-i}{\hbar} \right) \int_{t_0}^t dt' e^{i\omega_{ni}(t'-t_0)} V_{ni}(t')$$

$$c_n(t) = \langle n | \psi(t) \rangle_I = \langle n | U_I(t, t_0) | i \rangle$$

Análogamente:

$$c_n^{(2)}(t) = \left(\frac{-i}{\hbar} \right)^2 \sum_m \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' e^{i\omega_{nm}(t'-t_0)} V_{nm}(t') e^{i\omega_{mi}(t''-t_0)} V_{mi}(t'')$$

La probabilidad de encontrar a la partícula en el estado $|n\rangle$ es (si $n \neq i$)

$$\mathcal{P}_{i \rightarrow n}(t) = |c_n^{(1)}(t) + c_n^{(2)}(t) + \dots|^2 \quad (5.6.19)$$

Probabilidad de transición entre niveles del H_0

Perturbación constante

Perturbación constante

Supongamos que se enciende un potencial constante a $t=0$:

$$V(t) = \begin{cases} 0, & \text{for } t < 0 \\ V & \text{(independent of } t), \text{ for } t \geq 0. \end{cases}$$

Suponemos estado inicial $|\psi(0)\rangle_I = |i\rangle$

$$c_n^{(0)} = c_n^{(0)}(0) = \delta_{in}$$

$$c_n^{(1)} = \frac{-i}{\hbar} V_{ni} \int_0^t e^{i\omega_{ni}t'} dt' = \frac{V_{ni}}{E_n - E_i} (1 - e^{i\omega_{ni}t})$$

$$|c_n^{(1)}|^2 = \frac{|V_{ni}|^2}{|E_n - E_i|^2} (2 - 2\cos \omega_{ni}t) = \frac{4|V_{ni}|^2}{|E_n - E_i|^2} \sin^2 \left[\frac{(E_n - E_i)t}{2\hbar} \right]$$

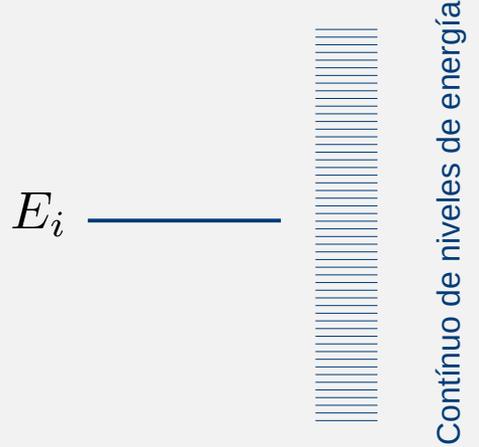
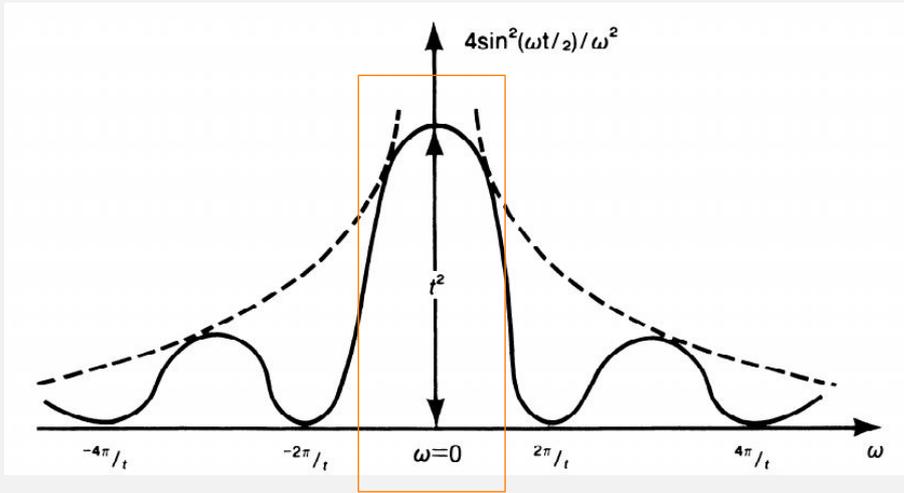
$$(1 - e^{i\omega_{ni}t})(1 - e^{-i\omega_{ni}t}) = 1 - e^{i\omega_{ni}t} - e^{-i\omega_{ni}t} + 1 = 2 - \cos(\omega_{ni}t)$$

Perturbación constante

$$|c_n^{(1)}|^2 = \frac{4|V_{ni}|^2}{|E_n - E_i|^2} \sin^2 \left[\frac{(E_n - E_i)t}{2\hbar} \right]$$

$$\omega \equiv \frac{E_n - E_i}{\hbar}$$

Miremos esta probabilidad de transición en función de la diferencia de energía a un dado tiempo t:



$$\Delta t \Delta E \sim \hbar$$

$$t \sim \frac{2\pi}{|\omega|} = \frac{2\pi\hbar}{|E_n - E_i|}$$

Perturbación constante

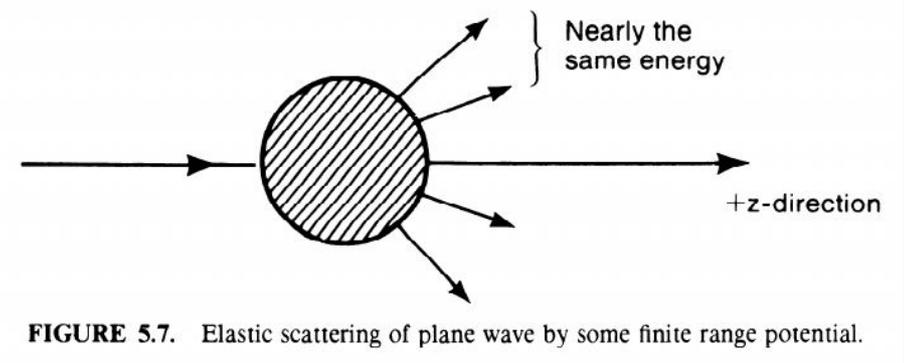


FIGURE 5.7. Elastic scattering of plane wave by some finite range potential.

Problemas de scattering

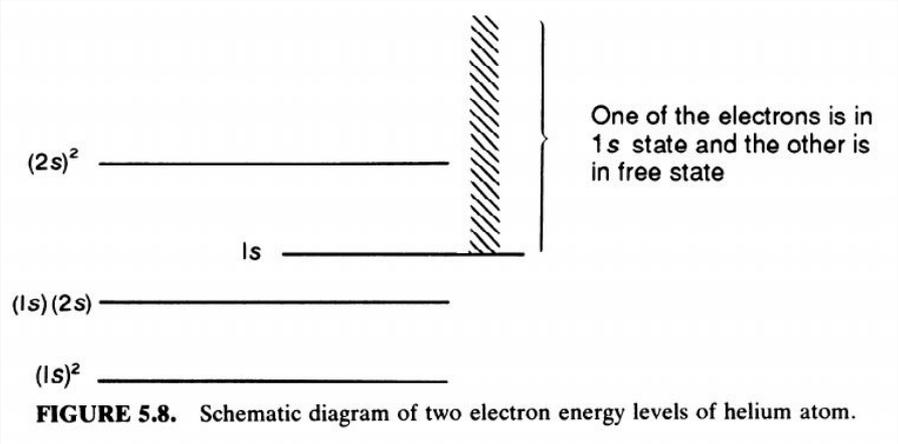
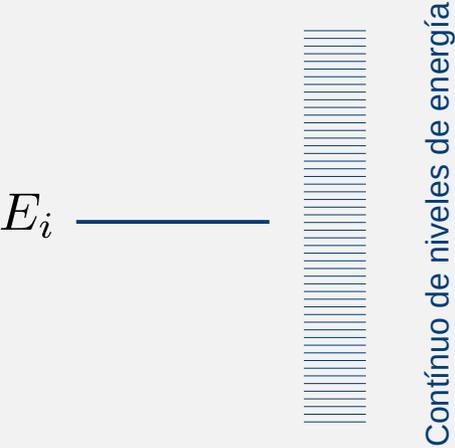


FIGURE 5.8. Schematic diagram of two electron energy levels of helium atom.



Densidad de estados:

$$\rho(E)dE$$

$$(E, E + dE)$$

Ionización por efecto Auger en átomos con más de un electrón

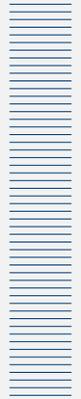
Perturbación constante

$$|c_n^{(1)}|^2 = \frac{4|V_{ni}|^2}{|E_n - E_i|^2} \sin^2 \left[\frac{(E_n - E_i)t}{2\hbar} \right]$$

Suponiendo que hay un continuo de energías disponibles,
tomando el límite $E_n \longrightarrow E_i$

$$|c_n^{(1)}(t)|^2 = \frac{1}{\hbar^2} |V_{ni}|^2 t^2$$

E_i —————



Continuo de niveles de energía

Ahora, en lugar de considerar un solo estado final consideremos la **probabilidad total de transición a otros estados** (cercanos a E_i)

$$\sum_{n, E_n \sim E_i} |c_n^{(1)}|^2$$

Regla de Oro de Fermi

Probabilidad total de transición a otros estados (cercanos a E_i)

Usando la densidad de estados $\rho(E)dE$:

$$\sum_{n, E_n \approx E_i} |c_n^{(1)}|^2 \Rightarrow \int dE_n \rho(E_n) |c_n^{(1)}|^2$$

$$= 4 \int \sin^2 \left[\frac{(E_n - E_i)t}{2\hbar} \right] \frac{|V_{ni}|^2}{|E_n - E_i|^2} \rho(E_n) dE_n$$

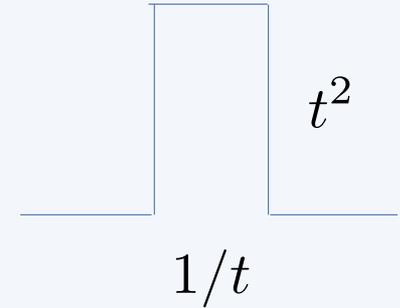
Usamos la propiedad de la delta de Dirac:

$$\lim_{\alpha \rightarrow \infty} \frac{1}{\pi} \frac{\sin^2 \alpha x}{\alpha x^2} = \delta(x)$$

$$\lim_{t \rightarrow \infty} \frac{1}{|E_n - E_i|^2} \sin^2 \left[\frac{(E_n - E_i)t}{2\hbar} \right] = \frac{\pi t}{2\hbar} \delta(E_n - E_i)$$

$$\lim_{t \rightarrow \infty} \int dE_n \rho(E_n) |c_n^{(1)}(t)|^2 = \left(\frac{2\pi}{\hbar} \right) |V_{ni}|^2 \rho(E_n) t \Big|_{E_n = E_i}$$

Transition rate (tasa de transición):



$$\frac{d}{dt} \left(\sum_n |c_n^{(1)}|^2 \right) = w_{i \rightarrow n} = \left(\frac{2\pi}{\hbar} \right) |V_{ni}|^2 \delta(E_n - E_i) \quad (5.6.34)$$

This formula is of great practical importance; it is called **Fermi's golden rule** even though the basic formalism of t -dependent perturbation theory is due to Dirac.* We sometimes write (5.6.34) as

$$w_{i \rightarrow n} = \left(\frac{2\pi}{\hbar} \right) |V_{ni}|^2 \delta(E_n - E_i), \quad (5.6.35)$$

where it must be understood that this expression is integrated with $\int dE_n \rho(E_n)$.

Perturbación armónica

$$V(t) = \mathcal{V} e^{i\omega t} + \mathcal{V}^\dagger e^{-i\omega t}$$

$$\begin{aligned} c_n^{(1)} &= \frac{-i}{\hbar} \int_0^t (\mathcal{V}_{n_i} e^{i\omega t'} + \mathcal{V}_{n_i}^\dagger e^{-i\omega t'}) e^{i\omega_{n_i} t'} dt' \\ &= \frac{1}{\hbar} \left[\frac{1 - e^{i(\omega + \omega_{n_i})t}}{\omega + \omega_{n_i}} \mathcal{V}_{n_i} + \frac{1 - e^{i(\omega_{n_i} - \omega)t}}{-\omega + \omega_{n_i}} \mathcal{V}_{n_i}^\dagger \right] \end{aligned}$$

Similar al caso de perturbación constante pero reemplazando:

$$\omega_{n_i} = \frac{E_n - E_i}{\hbar} \rightarrow \omega_{n_i} \pm \omega$$

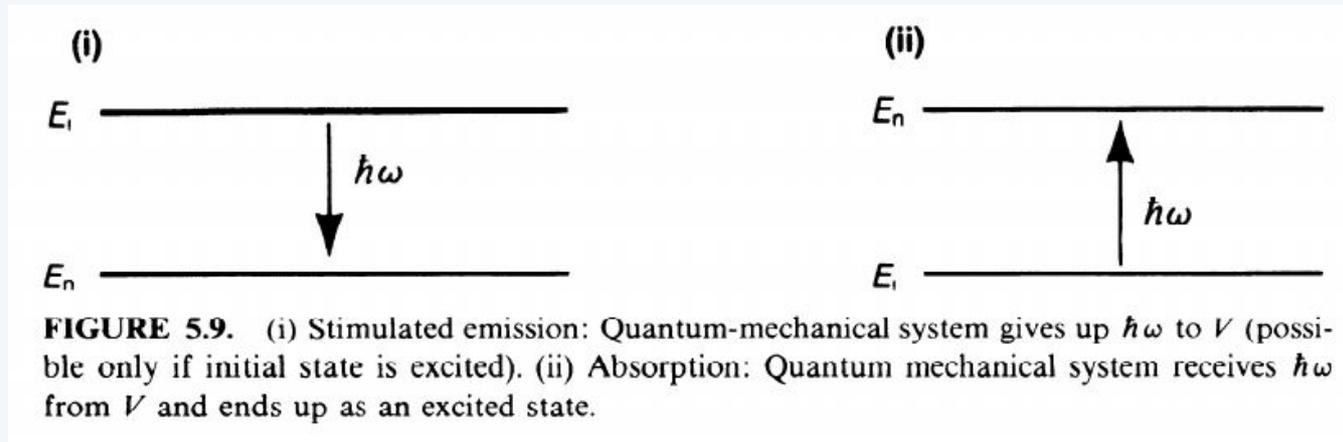
Hay transiciones con $t \rightarrow \infty$ si:

$$\omega_{ni} + \omega \simeq 0 \quad \text{or} \quad E_n \simeq E_i - \hbar\omega$$

Emisión estimulada

$$\omega_{ni} - \omega \simeq 0 \quad \text{or} \quad E_n \simeq E_i + \hbar\omega.$$

Absorción



Ahora se obtiene:

$$w_{i \rightarrow n} = \frac{2\pi}{\hbar} \left\{ \begin{array}{l} |\mathcal{V}_{ni}|^2 \\ |\mathcal{V}_{ni}^\dagger|^2 \end{array} \right\} \delta(E_n - E_i \pm \hbar\omega)$$

Resumen de la Clase 23

En esta clase vimos:

- Probabilidad de transición
- Tratamiento perturbativo dependiente del tiempo
- Perturbación constante
- Regla de oro de Fermi