

Martes 06/10/2020

La clase pasada vimos:

Propiedades de la **función de Green** de una partícula:
consecuencias de las invariancias temporal y traslacional

Ejemplo: función de Green del sistema de **fermiones libres**
y no-interactuantes

$$H \neq H(t) \Rightarrow G(\lambda t, \lambda' t') = G(\lambda(t - t'), \lambda' 0)$$

$t > t'$: Se **crea** una partícula en x' , las $N+1$ partículas evolucionan de t' a t , se **destruye** una partícula en x y se calcula el overlap con el ground state.

$$[\hat{H}, \hat{\mathbf{P}}] = 0 \Rightarrow G_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') = G((\mathbf{r} - \mathbf{r}')t, 0t)$$

$$[\hat{H}, \hat{\mathbf{P}}] = 0 \Rightarrow G_{\alpha\beta}(\mathbf{k}t, \mathbf{k}'t') = \delta_{\mathbf{k}, \mathbf{k}'} G_{\alpha\beta}(\mathbf{k}, t, t')$$

Ejemplo: fermiones libres y no interactuantes: $H_0 = T \quad V \equiv 0$

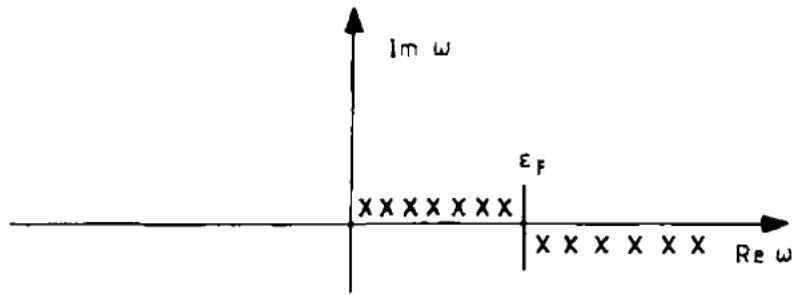
Funciones de Green

REPASO

$$iG_{\alpha\beta}^{(0)}(\mathbf{r}t, \mathbf{r}'t') = \delta_{\alpha\beta} \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} e^{-i\epsilon_k(t-t')} \\ \times [\theta(t-t')\theta(k-k_F) - \theta(t'-t)\theta(k_F-k)]$$

$$iG_{\alpha\beta}^{(0)}(\mathbf{k}, t-t') = \delta_{\alpha\beta} e^{-i\epsilon_k(t-t')} [\theta(t-t')\theta(k-k_F) - \theta(t'-t)\theta(k_F-k)]$$

$$\theta(\tau) = \lim_{\eta \rightarrow 0^+} -\frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega\tau}}{\omega + i\eta}$$



$$G_{\alpha\beta}^{(0)}(\mathbf{k}\omega) = \lim_{\eta \rightarrow 0^+} \delta_{\alpha\beta} \left[\frac{\theta(k-k_F)}{\omega - \epsilon_k + i\eta} + \frac{\theta(k_F-k)}{\omega - \epsilon_k - i\eta} \right]$$

Relación con observables físicos

La función de Green permite calcular:

1. El valor esperado de cualquier operador de una partícula en el estado fundamental.
2. La energía del estado fundamental (notar que la energía no está incluida en el punto anterior, o sea, no sale de un operador de una partícula si hay interacción).
3. El espectro de excitación del sistema.

Valor esperado de operador de una partícula en el estado fundamental

Sea un operador en Schrödinger: $\hat{A} = \sum_{i,j} \langle i|\hat{a}|j\rangle c_i^\dagger c_j$

Pasamos al picture de Heisenberg: $\hat{A}(t)_H = \sum_{i,j} \langle i|\hat{a}|j\rangle c_i^\dagger(t)_H c_j(t)_H$

Calculemos el valor medio del operador en el ground state exacto del sistema:

$$\langle \hat{A}(t) \rangle = \frac{\langle \Psi_0 | \hat{A}(t)_H | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} = \sum_{i,j} \langle i | \hat{a} | j \rangle \frac{\langle \Psi_0 | c_i^\dagger(t)_H c_j(t)_H | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

($|\Psi_0\rangle$ en Heisenberg)

$$= \lim_{t' \rightarrow t^+} \sum_{i,j} \langle i | \hat{a} | j \rangle \frac{\langle \Psi_0 | c_i^\dagger(t')_H c_j(t)_H | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

Tenemos :

$$\langle \hat{A}(t) \rangle = \lim_{t' \rightarrow t^+} \sum_{i,j} \langle i | \hat{a} | j \rangle \frac{\langle \Psi_0 | c_i^\dagger(t')_{\text{H}} c_j(t)_{\text{H}} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

Por definición de la función de Green:

$$iG(jt, it') = - \frac{\langle \Psi_0 | c_i^\dagger(t')_{\text{H}} c_j(t)_{\text{H}} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \quad \text{si } t' > t$$

Usando la notación matricial : $G(jt, it') = G_{ji}(t, t')$ tenemos :

$$\langle \hat{A}(t) \rangle = -i \lim_{t' \rightarrow t^+} \sum_{i,j} a_{ij} G_{ji}(t, t') = -i \lim_{t' \rightarrow t^+} \text{Tr}[\hat{a} G(t, t')]$$

$$\langle \hat{A}(t) \rangle = -i \text{Tr}[\hat{a} G(t, t^+)]$$

Traza del producto de matrices:

$$\left\{ \begin{array}{l} C_{ij} = \sum_k A_{ik} B_{kj} \\ \text{Tr}[C] = \sum_i C_{ii} = \sum_{i,k} A_{ik} B_{ki} \end{array} \right.$$

Mismo cálculo pero en la representación de espín-posición

Partimos del operador A en términos de los operadores de campo (lo suponemos local en las coordenadas espaciales):

$$A = \int d^3r \sum_{\beta\alpha} \psi_{\beta}^{\dagger}(\mathbf{r}) A_{\beta\alpha}(\mathbf{r}) \psi_{\alpha}(\mathbf{r})$$

Queremos estudiar el valor de expectación de A en el estado fundamental :

$$\langle A \rangle = \frac{1}{\langle \Psi_0 | \Psi_0 \rangle} \int d^3r \sum_{\alpha\beta} \langle \Psi_0 | \psi_{\beta}^{\dagger}(\mathbf{r}) A_{\alpha\beta}(\mathbf{r}) \psi_{\alpha}(\mathbf{r}) | \Psi_0 \rangle$$

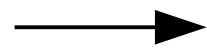
El operador $A_{\alpha\beta}(\mathbf{r})$ puede contener derivadas con respecto a \mathbf{r} , por eso adoptamos la notación :

$$\langle A \rangle = \frac{1}{\langle \Psi_0 | \Psi_0 \rangle} \int d^3r \lim_{\mathbf{r}' \rightarrow \mathbf{r}} \sum_{\alpha\beta} A_{\beta\alpha} \langle \Psi_0 | \psi_{\beta}^{\dagger}(\mathbf{r}') \psi_{\alpha}(\mathbf{r}) | \Psi_0 \rangle$$

Pasamos a la representación de Heisenberg :

$$\begin{aligned}
 & \langle \Psi_0 | \psi_\beta^\dagger(\mathbf{r}') \psi_\alpha(\mathbf{r}) | \Psi_0 \rangle \\
 &= \lim_{t' \rightarrow t} e^{-iE_0(t-t')} \langle \Psi_0 | \Psi_\beta^\dagger(\mathbf{r}') e^{iH(t-t')} \psi_\alpha(\mathbf{r}) | \Psi_0 \rangle \\
 &= \lim_{t' \rightarrow t} \langle \Psi_0 | \psi_\beta^\dagger(\mathbf{r}'t')_H \psi_\alpha(\mathbf{r}t)_H | \Psi_0 \rangle \\
 &= - \lim_{\substack{t' \rightarrow t \\ t' > t}} \langle \Psi_0 | T[\psi_\alpha(\mathbf{r}t)_H \psi_\beta^\dagger(\mathbf{r}'t')_H] | \Psi_0 \rangle \\
 &= - \lim_{t' \rightarrow t^+} iG_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') \langle \Psi_0 | \Psi_0 \rangle.
 \end{aligned}$$

Teníamos: $\langle A \rangle = \frac{1}{\langle \Psi_0 | \Psi_0 \rangle} \int d^3r \lim_{r' \rightarrow r} \sum_{\alpha\beta} A_{\beta\alpha} \langle \Psi_0 | \psi_\beta^\dagger(\mathbf{r}') \psi_\alpha(\mathbf{r}) | \Psi_0 \rangle$



$$\begin{aligned}
 \langle A \rangle &= -i \int d^3r \lim_{r' \rightarrow r} \lim_{t' \rightarrow t^+} \left[\sum_{\alpha\beta} A_{\beta\alpha}(\mathbf{r}) G_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') \right] \\
 &= -i \int d^3r \lim_{r' \rightarrow r} \text{Tr} (A(\mathbf{r}) G(\mathbf{r}t, \mathbf{r}'t^+)).
 \end{aligned}$$

$$\langle \hat{A}(t) \rangle = -i \text{Tr}[\hat{a} G(t, t^+)]$$

$$\langle \hat{A}(t) \rangle = -i \lim_{t' \rightarrow t^+} \sum_{i,j} a_{ij} G_{ji}(t, t') = -i \lim_{t' \rightarrow t^+} \text{Tr}[\hat{a} G(t, t')]$$

$$\begin{aligned} \langle A \rangle &= -i \int d^3r \lim_{\mathbf{r}' \rightarrow \mathbf{r}} \lim_{t' \rightarrow t^+} \left[\sum_{\alpha\beta} A_{\beta\alpha}(\mathbf{r}) G_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') \right] \\ &= -i \int d^3r \lim_{\mathbf{r}' \rightarrow \mathbf{r}} \text{Tr} (A(\mathbf{r}) G(\mathbf{r}t, \mathbf{r}'t^+)) . \end{aligned}$$

Traza en el spin

Funciones de Green

EJEMPLOS

$$\langle A \rangle = -i \int d^3r \lim_{r' \rightarrow r} \lim_{t' \rightarrow t^+} \left[\sum_{\alpha\beta} A_{\beta\alpha}(\mathbf{r}) G_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') \right]$$

$$= -i \int d^3r \lim_{r' \rightarrow r} \text{Tr} (A(\mathbf{r}) G(\mathbf{r}t, \mathbf{r}'t^+)).$$

(1) Energía cinética

$$T = \sum_{i=1}^N -\frac{\nabla_i^2}{2m} \quad \longrightarrow \quad \langle T \rangle = -i \int d^3r \lim_{r' \rightarrow r} \left(-\frac{\nabla_r^2}{2m} \right) \text{Tr} (G(\mathbf{r}t, \mathbf{r}'t^+))$$

(2) Operador densidad

$$\hat{\rho}(\mathbf{R}) = \sum_{i=1}^N \delta(\mathbf{R} - \mathbf{r}_i)$$

$$\rho(\mathbf{R}) = \langle \hat{\rho}(\mathbf{R}) \rangle = -i \int d^3r \lim_{r' \rightarrow r} \delta(\mathbf{R} - \mathbf{r}) \text{Tr} (G(\mathbf{r}t, \mathbf{r}'t^+))$$

$$= -i \int d^3r \delta(\mathbf{R} - \mathbf{r}) \text{Tr} (G(\mathbf{r}t, \mathbf{r}'t^+)) \quad \longleftarrow \quad \text{error: detectarlo}$$

$$= -i \text{Tr} (G(\mathbf{R}t, \mathbf{R}t^+)) = -i [G_{\uparrow\uparrow}(\mathbf{R}t, \mathbf{R}t^+) + G_{\downarrow\downarrow}(\mathbf{R}t, \mathbf{R}t^+)]$$

Funciones de Green

EJEMPLOS

$$\begin{aligned}\langle A \rangle &= -i \int d^3r \lim_{r' \rightarrow r} \lim_{t' \rightarrow t^+} \left[\sum_{\alpha\beta} A_{\beta\alpha}(\mathbf{r}) G_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') \right] \\ &= -i \int d^3r \lim_{r' \rightarrow r} \text{Tr} (A(\mathbf{r}) G(\mathbf{r}t, \mathbf{r}'t^+)).\end{aligned}$$

(3) Densidad de energía cinética

$$\hat{\tau}(\mathbf{R}) = \sum_{i=1}^N \delta(\mathbf{R} - \mathbf{r}_i) \left(-\frac{\nabla_i^2}{2m} \right)$$

$$\longrightarrow \tau(\mathbf{R}) = \langle \hat{\tau}(\mathbf{R}) \rangle = -i \lim_{r' \rightarrow r} \left(-\frac{\nabla_R^2}{2m} \right) \text{Tr} (G(\mathbf{R}t, \mathbf{r}'t'))$$

(4) Densidad de spin

$$\vec{\sigma}(\mathbf{R}) = \sum_{i=1}^N \delta(\mathbf{R} - \mathbf{r}_i) \vec{\sigma}_i \longrightarrow \langle \vec{\sigma}(\mathbf{R}) \rangle = -i \text{Tr} (\vec{\sigma} G(\mathbf{R}t, \mathbf{R}t^+))$$

EJEMPLOS

(4) Densidad de spin

$$\vec{\sigma}(\mathbf{R}) = \sum_{i=1}^N \delta(\mathbf{R} - \mathbf{r}_i) \vec{\sigma}_i \quad \longrightarrow \quad \langle \vec{\sigma}(\mathbf{R}) \rangle = -i \text{Tr} (\vec{\sigma} G(\mathbf{R}t, \mathbf{R}t^+))$$

$$\begin{aligned} \langle \sigma_z \rangle(\mathbf{R}, t) &= -i [\sigma_{z,\uparrow\uparrow} G_{\uparrow\uparrow}(\mathbf{R}t, \mathbf{R}t^+) + \sigma_{z,\uparrow\downarrow} G_{\downarrow\uparrow}(\mathbf{R}t, \mathbf{R}t^+) + \\ &\quad \sigma_{z,\downarrow\uparrow} G_{\uparrow\downarrow}(\mathbf{R}t, \mathbf{R}t^+) + \sigma_{z,\downarrow\downarrow} G_{\downarrow\downarrow}(\mathbf{R}t, \mathbf{R}t^+)] \\ &= -\frac{i\hbar}{2} [G_{\uparrow\uparrow}(\mathbf{R}t, \mathbf{R}t^+) - G_{\downarrow\downarrow}(\mathbf{R}t, \mathbf{R}t^+)] \end{aligned}$$

$$\langle \sigma_x \rangle(\mathbf{R}, t) = -\frac{i\hbar}{2} [G_{\downarrow\uparrow}(\mathbf{R}t, \mathbf{R}t^+) + G_{\uparrow\downarrow}(\mathbf{R}t, \mathbf{R}t^+)]$$

$$\langle \sigma_y \rangle(\mathbf{R}, t) = -\frac{i\hbar}{2} [-iG_{\downarrow\uparrow}(\mathbf{R}t, \mathbf{R}t^+) + iG_{\uparrow\downarrow}(\mathbf{R}t, \mathbf{R}t^+)]$$

Funciones de Green

$$\langle \hat{A}(t) \rangle = -i \lim_{t' \rightarrow t^+} \sum_{i,j} a_{ij} G_{ji}(t, t') = -i \lim_{t' \rightarrow t^+} \text{Tr}[\hat{a} G(t, t')]$$

Apliquemoslo a la **energía cinética del gas de electrones libres**.

Teníamos:


$$iG_{\alpha\beta}^{(0)}(\mathbf{k}, t - t') = \delta_{\alpha\beta} e^{-i\epsilon_{\mathbf{k}}(t-t')} [\theta(t-t')\theta(k - k_F) - \theta(t'-t)\theta(k_F - k)]$$

Entonces nos conviene trabajar en la base $|\mathbf{k}, \alpha\rangle$:

$$\langle A \rangle = -i \lim_{t' \rightarrow t^+} \sum_{\alpha, \beta} \sum_{\mathbf{k}, \mathbf{k}'} a_{\mathbf{k}'\beta, \mathbf{k}\alpha} G_{\alpha\beta}(\mathbf{k}t, \mathbf{k}'t')$$


Y usamos que:

$$G_{\alpha\beta}^{(0)}(\mathbf{k}t, \mathbf{k}'t') = \delta_{\alpha, \beta} \delta_{\mathbf{k}, \mathbf{k}'} G_{\alpha\alpha}(\mathbf{k}, t - t')$$


$$\langle A \rangle = -i \lim_{t' \rightarrow t^+} \sum_{\alpha} \sum_{\mathbf{k}} a_{\mathbf{k}\alpha, \mathbf{k}\alpha} G_{\alpha\alpha}(\mathbf{k}, t - t')$$

$$\langle A \rangle = -i \lim_{t' \rightarrow t^+} \sum_{\alpha} \sum_{\mathbf{k}} a_{\mathbf{k}\alpha, \mathbf{k}\alpha} G_{\alpha\alpha}(\mathbf{k}, t - t')$$

$$a_{\mathbf{k}\alpha, \mathbf{k}\alpha} = \frac{\hbar^2 k^2}{2m}$$

$$iG_{\alpha\beta}^{(0)}(\mathbf{k}, t - t') = \delta_{\alpha\beta} e^{-i\epsilon_{\mathbf{k}}(t-t')} [\theta(t-t')\theta(k-k_F) - \theta(t'-t)\theta(k_F-k)]$$

= 1 en el limite $t' \rightarrow t^+$

Entonces:
$$\langle A \rangle = 2i \lim_{t' \rightarrow t^+} \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m} (-i)\theta(t-t')\theta(k_F-k)$$

$$\langle A \rangle = 2 \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m} \theta(k_F - k) = \frac{3}{5} \frac{\hbar^2 k_F^2}{2m}$$

Funciones de Green

Energía del estado fundamental (valor de expectación de H en el GS)

$$E_0 = -\frac{i}{2} \int d^3r \lim_{t' \rightarrow t} \lim_{\mathbf{r}' \rightarrow \mathbf{r}} \left(i \frac{\partial}{\partial t} - \frac{\nabla_{\mathbf{r}}^2}{2m} \right) \text{Tr} [G_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t')] . \quad (15.20)$$

Demostración

Consideremos un Hamiltoniano de la forma:

$$H = T + V = \sum_{\alpha} \int d^3r \psi_{\alpha}^{\dagger}(\mathbf{r}) \left(-\frac{\nabla_{\mathbf{r}}^2}{2m} \right) \psi_{\alpha} \\ + \frac{1}{2} \sum_{\substack{\alpha\alpha' \\ \beta\beta'}} \int \int d^3r d^3r' \psi_{\alpha}^{\dagger}(\mathbf{r}) \psi_{\beta}^{\dagger}(\mathbf{r}') V_{\beta\beta'}^{\alpha\alpha'}(\mathbf{r}, \mathbf{r}') \psi_{\beta'}(\mathbf{r}') \psi_{\alpha'}(\mathbf{r})$$

(Permitimos una dependencia general, no-diagonal, en spin.)

Habría que demostrar el siguiente conmutador :

$$[\psi_{\alpha}(\mathbf{r}), H] = -\frac{\nabla_{\mathbf{r}}^2}{2m}\psi_{\alpha}(\mathbf{r}) + \sum_{\alpha'\beta\beta'} \int d^3\mathbf{y} \psi_{\beta}^{\dagger}(\mathbf{y}) V_{\alpha\alpha'}_{\beta\beta'}(\mathbf{r}, \mathbf{y}) \psi_{\beta'}(\mathbf{y}) \psi_{\alpha'}(\mathbf{r})$$

que nos permite obtener la ecuación de movimiento de Heisenberg del operador de campo :

$$\begin{aligned} i\frac{\partial}{\partial t}\psi_{\alpha}(\mathbf{r}t)_H &= [\psi_{\alpha}(\mathbf{r}t)_H, H] = e^{iHt} [\psi_{\alpha}(\mathbf{r})_S, H] e^{-iHt} \\ &= \left[-\frac{\nabla_{\mathbf{r}}^2}{2m} \right] \psi_{\alpha}(\mathbf{r}t)_H \\ &\quad + \sum_{\alpha'\beta\beta'} \int d^3\mathbf{y} \psi_{\beta}^{\dagger}(\mathbf{y}t)_H V_{\alpha\alpha'}_{\beta\beta'}(\mathbf{r}, \mathbf{y}) \psi_{\beta'}(\mathbf{y}t)_H \psi_{\alpha'}(\mathbf{r}t)_H \end{aligned}$$

$$\begin{aligned}
 i \frac{\partial}{\partial t} \psi_{\alpha}(\mathbf{r}t)_H &= [\psi_{\alpha}(\mathbf{r}t)_H, H] = e^{iHt} [\psi_{\alpha}(\mathbf{r})_S, H] e^{-iHt} \\
 &= \left[-\frac{\nabla_{\mathbf{r}}^2}{2m} \right] \psi_{\alpha}(\mathbf{r}t)_H \\
 &\quad + \sum_{\alpha' \beta \beta'} \int d^3 \mathbf{y} \psi_{\beta}^{\dagger}(\mathbf{y}t)_H V_{\alpha \alpha'}_{\beta \beta'}(\mathbf{r}, \mathbf{y}) \psi_{\beta'}(\mathbf{y}t)_H \psi_{\alpha'}(\mathbf{r}t)_H
 \end{aligned}$$

Aplicamos $\psi_{\alpha}^{\dagger}(\mathbf{r}'t')_H$ a izquierda, tomamos valor medio $\langle \Psi_0 | \dots | \Psi_0 \rangle$

y normalizamos 

$$\begin{aligned}
 &\left[i \frac{\partial}{\partial t} - \left(-\frac{\nabla_{\mathbf{r}}^2}{2m} \right) \right] \frac{\langle \Psi_0 | \psi_{\alpha}^{\dagger}(\mathbf{r}'t')_H \psi_{\alpha}(\mathbf{r}t)_H | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \\
 &= \sum_{\alpha' \beta \beta'} \int d^3 \mathbf{y} \frac{1}{\langle \Psi_0 | \Psi_0 \rangle} \\
 &\quad \times \langle \Psi_0 | \psi_{\alpha}^{\dagger}(\mathbf{r}'t')_H \psi_{\beta}^{\dagger}(\mathbf{y}t)_H V_{\alpha \alpha'}_{\beta \beta'}(\mathbf{r}, \mathbf{y}) \psi_{\beta'}(\mathbf{y}t)_H \psi_{\alpha'}(\mathbf{r}t)_H | \Psi_0 \rangle
 \end{aligned}$$

$$\begin{aligned} & \left[i \frac{\partial}{\partial t} - \left(-\frac{\nabla_{\mathbf{r}}^2}{2m} \right) \right] \frac{\langle \Psi_0 | \psi_{\alpha}^{\dagger}(\mathbf{r}'t')_H \psi_{\alpha}(\mathbf{r}t)_H | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \\ &= \sum_{\alpha' \beta \beta'} \int d^3 y \frac{1}{\langle \Psi_0 | \Psi_0 \rangle} \\ & \quad \times \langle \Psi_0 | \psi_{\alpha}^{\dagger}(\mathbf{r}'t')_H \psi_{\beta}^{\dagger}(\mathbf{y}t)_H V_{\beta\beta'}(\mathbf{r}, \mathbf{y}) \psi_{\beta'}(\mathbf{y}t)_H \psi_{\alpha'}(\mathbf{r}t)_H | \Psi_0 \rangle \end{aligned}$$

En el lado derecho podemos hacer aparecer $\langle \Psi_0 | V | \Psi_0 \rangle$

We now take the limits $\mathbf{r}' \rightarrow \mathbf{r}$ and $t' \rightarrow t$ in this equation, then integrate over $d^3 r$ and sum over α . From the definition of the single-particle Green's function it then follows that

$$\int d^3 r \lim_{t' \rightarrow t^+} \lim_{\mathbf{r}' \rightarrow \mathbf{r}} \left(i \frac{\partial}{\partial t} + \frac{\nabla_{\mathbf{r}}^2}{2m} \right) \text{Tr} [-i G_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t')] = 2 \langle \Psi_0 | V | \Psi_0 \rangle.$$

Continuará