GREEN FUNCTIONS

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1. The propagator

In quantum mechanics, the time evolution in Hilbert space $\mathscr{H}$ is assigned by a family of unitary operators (named *propagator*) $|\psi(t)\rangle = U(t,t')|\psi(t')\rangle$, with the natural property

$$U(t,t')U(t',t'') = U(t,t'') \tag{1}$$

and strong continuity in both time-arguments[1]. Note that $U(t,t) = 1$, $U(t,t')^\dagger = U(t',t)$. If θ is a fixed reference time, the following factorization provides the full propagator: $U(t,t') = U(t,\theta)U(t',\theta)^\dagger$.

A derivative in t of (1) and right multiplication by $U(t'',t)$ gives

$$[\partial_t U(t,t')]U(t',t) = [\partial_t U(t,t'')]U(t'',t)$$

which shows that $[\partial_t U(t,t')]U(t',t)$ is independent of t'. Next, the derivative of $U(t,t')U(t',t) = 1$ shows that $i\hbar[\partial_t U(t,t')]U(t',t)$ is self-adjoint and has the dimension of energy. Let's name the operator $H(t)$ (the Hamiltonian). The *Schrödinger equation* follows:

$$\boxed{i\hbar\partial_t U(t,t') = H(t)U(t,t')} \tag{2}$$

with initial condition $U(t',t') = I$.

• The time-evolution is stationary if $U(t+s,t'+s) = U(t,t')$ for all s,t,t'. The Hamiltonian is time-independent and $U(t,s) = e^{-\frac{i}{\hbar}(t-s)H}$.

• The time-evolution is periodic with period τ, if $U(t+\tau,t'+\tau) = U(t,t')$ for all t,t'. The *Floquet* operator $U(\tau,0)$ and $U(t,0)$ with $0 \le t < \tau$ reconstruct the whole propagator. The representation $U(\tau,0) = \exp(-iE\tau)$ defines the self-adjoint *quasi-energy* operator E, as important as H in stationary systems.

2. Some operator identities

A system of bosons or fermions is described by the Hamiltonian $H = H_1 + H_2$, where H_1 and H_2 are the one and two particle operators

$$H_1 = \sum_{ab} h_{ab} c_a^\dagger c_b, \qquad H_2 = \tfrac{1}{2}\sum_{abcd} v_{abcd} c_a^\dagger c_b^\dagger c_d c_c \tag{3}$$

An arbitrary one-particle basis is used, with corresponding canonical operators c_a and $c_a^\dagger$. The matrix elements are $h_{ab} = \langle a|h|b\rangle$ and $v_{abcd} = \langle ab|v|cd\rangle = v_{badc}$ (invariance for exchange of particles). The ground state of H is $|gs\rangle$.

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[1] see Reed-Simon, Functional analysis, p.282

The Heisenberg time-evolution of an operator governed by H is $O_H(t) = e^{iHt/\hbar} O e^{-iHt/\hbar}$. It solves the equation of motion

$$i\hbar \frac{d}{dt} O_H(t) = e^{iHt/\hbar}[O,H]e^{-iHt/\hbar}. \tag{4}$$

Let us evaluate $[c_r, H]$. By means of the *commutators*

$$[c_r, c_a^\dagger c_b] = \delta_{ar} c_b \tag{5}$$

$$[c_r, c_a^\dagger c_b^\dagger c_d c_c] = (\delta_{ra} c_b^\dagger \pm \delta_{rb} c_a^\dagger) c_d c_c \tag{6}$$

we obtain $[c_r, H_1] = \sum_b h_{rb} c_b$ and $[c_r, H_2] = \frac{1}{2}\sum_{bcd}(v_{rbcd} \pm v_{brcd}) c_b^\dagger c_d c_c$. The indices c and d are exchanged in the second term; next the destruction operators are exchanged: $c_c c_d = \pm c_d c_c$. Then $[c_r, H_2] = \frac{1}{2}\sum_{bcd}(v_{rbcd} + v_{brdc}) c_b^\dagger c_d c_c$. Since $\langle ab|v|cd\rangle = \langle ba|v|dc\rangle$, the final expression is obtained:

$$\boxed{[c_r, H] = \sum_b h_{rb} c_b + \sum_{bcd} v_{rbcd} c_b^\dagger c_d c_c} \tag{7}$$

The following algebraic identities are useful, and simple to obtain:

$$\sum_r c_r^\dagger [c_r, H] = H_1 + 2H_2 \tag{8}$$

$$[c_r^\dagger, H] = -\sum_a c_a^\dagger h_{ar} - \sum_{abc} v_{abrc} c_a^\dagger c_b^\dagger c_c \tag{9}$$

$$i\hbar \frac{d}{dt} c_r(t) = \sum_b h_{rb} c_b(t) + \sum_{bcd} v_{rbcd} (c_b^\dagger c_d c_c)(t) \tag{10}$$

3. The time-ordered Green function

Let us introduce the symbol T of *time-ordering of operators*. Its action on a product of creation/destruction operators of any set of states (we use a letter A), at *different* times of Heisenberg evolution with the Hamiltonian H, is to reorder them with times decreasing from left to right:

$$\mathsf{T} A_1(t_1) \dots A_N(t_N) = (\pm 1)^\sigma A_{\sigma_1}(t_{\sigma_1}) \dots A_{\sigma_N}(t_{\sigma_N}), \quad t_{\sigma_1} > \dots > t_{\sigma_N} \tag{11}$$

σ is the permutation that produces the time-ordered product: $+1$ for boson statistics, or ± 1 for Fermi statistics, according to the number of exchanges in σ being even or odd.

The definition implies that creation/destruction operators may be permuted under the symbol of T-ordering, up to a sign:

$$\mathsf{T} A_1(t_1) \dots A_N(t_N) = (\pm 1)^\sigma \mathsf{T} A_{\sigma_1}(t_{\sigma_1}) \dots A_{\sigma_N}(t_{\sigma_N}) \tag{12}$$

The action of T on a product of generic operators written in second quantization and at different times, is defined by linearity.

The 1-particle time-ordered Green function is:

$$\boxed{iG_{rr'}(t,t') = \langle gs|\mathsf{T} c_r(t) c_{r'}^\dagger(t')|gs\rangle} \tag{13}$$

If the action of T and the Heisenberg evolution are written explicitly, it is:

$$\begin{aligned} iG_{rr'}(t,t') &= \theta(t-t') e^{-\frac{i}{\hbar}E_{gs}(t'-t)} \langle gs|c_r U(t-t') c_{r'}^\dagger|gs\rangle \\ &\pm \theta(t'-t) e^{-\frac{i}{\hbar}E_{gs}(t-t')} \langle gs|c_{r'}^\dagger U(t'-t) c_r|gs\rangle \end{aligned}$$

where + is for bosons, and − for fermions.
The interpretation is simple. If $t > t'$, the matrix element $\langle gs|c_r U(t-t')c^\dagger_{r'}|gs\rangle$ is the projetion of the state $c^\dagger_{r'}|gs\rangle$ propagated in time $t-t'$, on the state $c^\dagger_r|gs\rangle$. States are not normalized: $\|c^\dagger_r|gs\rangle\|^2 = \langle gs|c_r c^\dagger_r|gs\rangle = 1 \pm n_r$. If the normalization is taken into account and if, for fermions, $n_r < 1$ and $n_{r'} < 1$,

$$|G_{r,r'}(t,t')|^2 = \frac{|\langle gs|c_r U(t-t')c^\dagger_{r'}|gs\rangle|^2}{(1\pm n_r)(1\pm n_{r'})}$$

is the probability that a particle created in a state r', is observed in a state r after a time $t-t'$, indistiguishable from the particles in the ground state.

The time-ordered Green function depends on the difference $t-t'$ and is discontinuous at $t-t'=0$:

$$\begin{aligned} iG_{r,r'}(t^+,t) - iG_{r,r'}(t^-,t) =& \langle gs|c_r(t)c^\dagger_{r'}(t) \mp c^\dagger_{r'}(t)c_r(t)|gs\rangle \\ =& \langle gs|c_r c^\dagger_{r'} \mp c^\dagger_{r'}c_r|gs\rangle = \langle r|r'\rangle \end{aligned}$$

It is advantageous to Fourier transform to frequency space:

$$G_{r,r'}(t,t') = \int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}G_{r,r'}(\omega)e^{-i\omega(t-t')} \tag{14}$$

With the knowledge of the Green function, the ground-state average of any 1-particle operator may be evaluated:

$$\langle gs|c^\dagger_r c_s|gs\rangle = \langle gs|c^\dagger_r(t^+)c_s(t)|gs\rangle = \langle gs|\mathsf{T}c^\dagger_r(t^+)c_s(t)|gs\rangle = \pm iG_{sr}(t,t^+)$$

$$\boxed{\langle O\rangle = \pm i\sum\nolimits_{rs} O_{rs}G_{sr}(t,t^+)} \tag{15}$$

For example, the ground-state average of the density of particles with spin m is:

$$\begin{aligned} n_m(\mathbf{x},t) = \langle gs|\psi^\dagger_m(\mathbf{x})\psi_m\mathbf{x})|gs\rangle =& \pm iG_{mm}(\mathbf{x},t;\mathbf{x},t^+) \\ =& \pm i\int\frac{d\omega}{2\pi}G_{mm}(\mathbf{x},\mathbf{x},\omega)e^{i\omega\eta} \end{aligned} \tag{16}$$

4. Green function of non-interacting fermions

Consider the Hamiltonian of non-interacting particles $H^0 = \sum_a \hbar\omega_a c^\dagger_a c_a$. This diagonal form results if the operators refer to the eigenstates of the single particle Hamiltonian $hu_a = \hbar\omega_a u_a$. States are ordered in increasing energy, $\hbar\omega_1 < \hbar\omega_2 \le ....$ For N particles the Fermi energy is that of the highest occupied state $\epsilon_F = \hbar\omega_F$.

The time evolutions are simple:

$$c_a(t) = e^{-i\omega_a t}c_a, \qquad c^\dagger_a(t) = e^{-i\omega_a t}c^\dagger_a$$

One evaluates:

$$\begin{aligned} iG^0_{mm'}(\mathbf{x},t;\mathbf{x}',t') =& \sum_{aa'}\langle\mathbf{x},m|a\rangle\langle a|\mathbf{x}',m'\rangle\langle gs|\mathsf{T}c_a(t)c^\dagger_{a'}(t')|gs\rangle \\ =& \sum_a\langle\mathbf{x},m|a\rangle\, e^{-i\omega_a(t-t')}\langle a|\mathbf{x}',m'\rangle \\ & \times[\theta(t-t')\theta(\omega_a-\omega_F) - \theta(t'-t)\theta(\omega_F-\omega_a)] \\ \equiv& i\int\frac{d\omega}{2\pi}G^0_{mm'}(\mathbf{x},\mathbf{x}',\omega)e^{-i\omega(t-t')} \end{aligned} \tag{17}$$

The identification of the Fourier transform requires the insertion of the Fourier expansions of the temporal theta functions,

$$\boxed{\theta(t-t') = i\int \frac{d\omega}{2\pi}\frac{e^{-i\omega(t-t')}}{\omega+i\eta}}$$

After shifts of variables the result is:

$$G^0_{mm'}(\mathbf{x},\mathbf{x}',\omega) = \sum_a \langle \mathbf{x}m|a\rangle\langle a|\mathbf{x}'m\rangle \left[\frac{\theta(\omega_a-\omega_F)}{\omega-\omega_a+i\eta} + \frac{\theta(\omega_F-\omega_a)}{\omega-\omega_a-i\eta}\right] \tag{18}$$

For the ideal gas of fermions $|a\rangle = |\mathbf{k}m\rangle$. One finds $G^0_{mm'}(\mathbf{k},\omega) = \delta_{mm'}G^0(\mathbf{k},\omega)$,

$$G^0(\mathbf{k},\omega) = \frac{\theta(\omega_k-\omega_F)}{\omega-\omega_k+i\eta} + \frac{\theta(\omega_F-\omega_k)}{\omega-\omega_k-i\eta} \tag{19}$$

$$= \frac{1}{\omega-\omega_k+i\eta\,\mathrm{sign}(\omega_k-\omega_F)} \tag{20}$$

where $\hbar\omega_k = \hbar^2k^2/2m$.

5. The ground state energy

The operator identity eq.(8) yields an expression for the total energy, due to **Galitskii** and **Migdal**.
First evolve the terms in time: $\sum_r c^\dagger_r(t)[c_r(t),H] = H_1(t)+2H_2(t)$ and use $[c_r(t),H] = i\hbar\dot{c}_r(t)$. Next take the expectation value on the exact ground state:

$$\langle gs|H_1(t)+2H_2(t)|gs\rangle = i\hbar\sum_r \langle gs|c^\dagger_r(t)\frac{d}{dt}c_r(t)|gs\rangle = i\hbar\lim_{t'\to t}\sum_r\frac{\partial}{\partial t}\langle gs|c^\dagger_r(t')c_r(t)|gs\rangle$$

For a single operator it is $\langle gs|O(t)|gs\rangle = \langle gs|e^{+\frac{i}{\hbar}Ht}Oe^{-\frac{i}{\hbar}Ht}|gs\rangle = \langle gs|O|gs\rangle$:

$$\langle gs|H_1+2H_2|gs\rangle = i\hbar\lim_{t'\to t}\sum_r\frac{\partial}{\partial t}\langle gs|c^\dagger_r(t')c_r(t)|gs\rangle$$

If $t'\ge t^+$ a T-ordering can be introduced in the inner product without any change. This allows to exchange the operators and obtain:

$$\langle gs|H_1+2H_2|gs\rangle = \mp\hbar\lim_{t'\to t^+}\frac{\partial}{\partial t}\sum_r G_{rr}(t,t')$$

The equation provides the expectation value of the 2-particle operator H_2 in terms of the 1-particle Green function[2]. The total energy is $E_{GS} = \langle H_1\rangle + \langle H_2\rangle$:

$$\boxed{E_{GS} = \pm\frac{i}{2}\lim_{t'\to t^+}\sum_{ab}\left[i\hbar\delta_{ab}\frac{\partial}{\partial t}+h_{ab}\right]G_{ba}(t,t')} \tag{21}$$

In frequency space:

$$E_{GS} = \pm\frac{i}{2}\sum_{ab}\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\left[\hbar\omega\delta_{ab}+h_{ab}\right]G_{ba}(\omega)e^{i\omega\eta} \tag{22}$$

In the basis of position and spin, and for a potential that does not depend on spin:

$$E_{GS} = \pm\frac{i}{2}\sum_m\int d^3x\left[i\hbar\frac{\partial}{\partial t}-\frac{\hbar^2}{2m}\nabla^2_{\mathbf{x}}+U(\mathbf{x})\right]G_{mm}(\mathbf{x}t,\mathbf{x}'t')\Big|_{(\mathbf{x}',t')=(\mathbf{x},t^+)}$$

[2] The single particle average is: $\langle H_1\rangle = \mp i\sum_{ab}h_{ab}G_{ba}(t,t^+)$.

In presence of translation invariance and spin independent interaction, the formula simplifies to

$$\frac{E_{gs}}{V} = \pm i\frac{(2s+1)}{2}\int \frac{d^3k\, d\omega}{(2\pi)^4}[\hbar\omega + \epsilon(\mathbf{k})]G(\mathbf{k},\omega)e^{i\omega\eta}$$

where V is the volume.

6. **Equation of motion of the propagator**

Let us evaluate

$$i\hbar\frac{\partial}{\partial t}G_{rr'}(t,t') = \hbar\frac{\partial}{\partial t}\left[\theta(t-t')\langle c_r(t)c^\dagger_{r'}(t')\rangle \pm \theta(t'-t)\langle c^\dagger_{r'}(t')c_r(t)\rangle\right]$$
$$= \hbar\delta(t-t')\langle c_r(t)c^\dagger_{r'}(t') \mp c^\dagger_{r'}(t')c_r(t)\rangle + \hbar\langle \mathsf{T}\frac{dc_r(t)}{dt}c^\dagger_{r'}(t')\rangle$$
$$= \hbar\delta(t-t')\delta_{rr'} - i\sum_b h_{rb}\langle \mathsf{T}c_b(t)c^\dagger_{r'}(t')\rangle - i\sum_{bcd} v_{rbcd}\langle \mathsf{T}\,(c^\dagger_b c_d c_c)(t)c^\dagger_{r'}(t')\rangle$$

$$\sum_b \left[\delta_{rb}i\hbar\frac{\partial}{\partial t} - h_{rb}\right]G_{br'}(t,t') = \hbar\delta(t-t')\delta_{rr'} - i\sum_{bcd} v_{rbcd}\langle \mathsf{T}\,(c^\dagger_b c_d c_c)(t)c^\dagger_{r'}(t')\rangle$$

In the last term, the T ordering acts on the triplet as a single operator at time t. To treat the three operators individually, the ambiguity of equal time is avoided by adding infinitesimal time shifts that keep memory of the original order:

$$\begin{aligned}\langle \mathsf{T}(c^\dagger_b c_d c_c)(t)c^\dagger_{r'}(t')\rangle &= \langle \mathsf{T}c^\dagger_b(t^{++})c_d(t^+)c_c(t)c^\dagger_{r'}(t')\rangle \\ &= \langle \mathsf{T}c_c(t)c_d(t^+)c^\dagger_{r'}(t')c^\dagger_b(t^{++})\rangle\end{aligned}$$

Inside a T product the operators may be permuted, up to a sign. The $++$ and $+$ must be left in place as far as T is present. The matrix element has been written with creation operators at the right, to comply with the definition of the two-particle Green function:

$$\boxed{i^2 G_{abcd}(t_a,t_b,t_c,t_d) = \langle \mathsf{T}c_a(t_a)c_b(t_b)c^\dagger_d(t_d)c^\dagger_c(t_c)\rangle} \tag{23}$$

(note the positions of labels c and d). Because of $\mathsf{T}-$ordering:

$$G_{abcd}(t_a,t_b,t_c,t_d) = \pm\, G_{bacd}(t_b,t_a,t_c,t_d) = \pm\, G_{abdc}(t_a,t_b,t_d,t_c) \tag{24}$$

The equation of motion of the propagator is obtained:

$$\sum_b (i\hbar\delta_{rb}\partial_t - h_{rb})G_{br'}(t,t') = \hbar\delta_{rr'}\delta(t-t') + i\sum_{bcd} v_{rbcd}G_{cdbr'}(t,t^+,t^{++},t') \tag{25}$$

It is the first equation in an infinite hierarchy, obtained by **Martin** and **Schwinger**, where each step involves higher order Green functions.
In the position representation, for spin-independent interactions, the equation is:

$$\begin{aligned}(i\hbar\partial_t - h(\mathbf{x}))\,G_{mm'}(\mathbf{x}t,\mathbf{x}'t') &= \hbar\delta_{mm'}\delta_3(\mathbf{x}-\mathbf{x}')\delta(t-t') \\ &+ i\sum_{m''}\int d^3y\; v(\mathbf{x},\mathbf{y})\,G_{mm''m''m'}(\mathbf{x}t,\mathbf{y}t^+,\mathbf{y}t^{++},\mathbf{x}'t')\end{aligned} \tag{26}$$

If the particles do not interact, the equation of motion does not involve the 2-particle Green function. Let us pause for a while on Green functions of non-interacting particles.

7. Independent particles

For non-interacting particles the Green function is a distribution solving

$$(\delta_{ab} i\hbar\partial_t - h_{ab})G^0_{bc}(t,t') = \hbar\delta_{ac}\delta(t-t') \tag{27}$$

The equation does not have a unique solution, as one may add a solution of the homogeneous problem. In frequency space it is $(\hbar\omega\delta_{ab} - h_{ab})G^0_{bc}(\omega) = \hbar\delta_{ac}$, which is recognized as the basis-projected equation for the resolvent operator:

$$(\hbar\omega - \hat{h})\,\hat{G}^0(\omega) = \hbar$$

with $G^0_{ab}(\omega) = \langle a|G^0(\omega)|b\rangle$. The resolvent $\hat{G}^0(\omega) = (\omega - \frac{1}{\hbar}\hat{h})^{-1}$ exists for $\hbar\omega$ not in the spectrum of $\hat{h}$. By assuming a discrete spectrum for $\hat{h}$:

$$G^0_{ab}(\omega) = \sum_j \frac{\langle a|j\rangle\langle j|b\rangle}{\omega - \frac{1}{\hbar}\epsilon_j}$$

To make sense of the Fourier integral for $G^0_{ab}(t,t')$ one shifts poles (and cuts) off the real axis by infinitesimal amounts. This can be done in various ways, leading to Green functions that differ by solutions of the homogeneous equation. The most useful ones are the *retarded* and the *time-ordered* Green functions.

The retarded Green function The whole spectrum of $\hat{h}$ is shifted to the lower half of the $\omega-$plane by an infinitesimal amount:

$$G^{0R}_{ab}(\omega) =: \sum_j \frac{\langle a|j\rangle\langle j|b\rangle}{\omega - \frac{1}{\hbar}\epsilon_j + i\eta} \tag{28}$$

In passing we note that the imaginary part of the diagonal matrix elements give the *weighted density of states*:

$$-\frac{1}{\pi}\mathrm{Im}\, G^{0R}_{a,a}(\omega) =: \sum_j |\langle a|j\rangle|^2\delta(\omega - \tfrac{1}{\hbar}\epsilon_j) \tag{29}$$

The trace (which is basis-independent) is the density of states of the Hamiltonian:

$$-\frac{1}{\pi}\mathrm{Im}\,\mathrm{tr}\, G^{0R}(\omega) =: \sum_j \delta(\omega - \tfrac{1}{\hbar}\epsilon_j)$$

Consider the inhomogeneous equation $[i\hbar\delta_{ab}\partial_t - h_{ab}]f_b(t) = g_a(t)$ with unknown functions $f_a(t)$ and assigned sources $g_a(t)$. The general solution can be obtained with the aid of the Green function:

$$f_a(t) = f^0_a(t) + \frac{1}{\hbar}\int dt' \sum\nolimits_b G^0_{ab}(t,t')g_b(t');$$

where $f^0_a(t)$ solves the homogeneus equation.

Since the retarded Green function is analytic in the upper half plane, its Fourier transform to the time variables is zero for $t' > t$, by the residue theorem,

$$\begin{aligned} G^{0R}_{ab}(t,t') &= \int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}e^{-i\omega(t-t')}G^R_{ab}(\omega) \\ &= -i\,\theta(t-t')\sum_n e^{-i\omega_n(t-t')}\langle a|n\rangle\langle n|b\rangle \\ &= -i\,\theta(t-t')\,\langle a|U(t,t')|b\rangle \end{aligned}$$

This feature is of great importance in physics as it expresses *causality*: the particular solution

$$f_a^R(t) = \int dt\, G_{ab}^{0R}(t,t')\, g_b(t')$$

only depends on the values of the source $g(t')$ at earlier times $t' < t$.

In a many body system, the retarded Green function is the expectation value of the commutator (bosons) or anticommutator (fermions) at unequal times. The definition holds also for interacting systems:

$$\boxed{iG_{ab}^R(t,t') = \theta(t-t')\, \langle gs|\left[c_a(t), c_b^\dagger(t')\right]_\mp |gs\rangle} \tag{30}$$

Exercise 1. *Evaluate the retarded Green function for free particles* $G^{0R}(\mathbf{x}, t; \mathbf{x}', t')$ *(the result does not depend on statistics).*

The time-ordered Green function - fermions. In the time ordered Green function the Fermi frequency divides the spectrum into a portion that gains a positive imaginary part and another that gains a negative imaginary correction:

$$G_{ab}^{0T}(\omega) =: \sum_j \frac{\langle a|u_j\rangle\langle u_j|b\rangle}{\omega - \frac{1}{\hbar}\epsilon_j + i\eta\, \mathrm{sign}(\epsilon_j - \epsilon_F)} \tag{31}$$

If states are ordered according to increasing energies, ϵ_F is the highest energy available for N fermions in the ground state.
The Fourier transform to time variables is (in position-spin basis)

$$\begin{aligned} iG_{mm'}^{0T}(\mathbf{x}, t; \mathbf{x}', t') = &\sum_j e^{-\frac{i}{\hbar}\epsilon_j(t-t')}\langle \mathbf{x}m|u_j\rangle\langle u_j|\mathbf{x}'m'\rangle \\ &\times [\theta(t-t')\theta(\epsilon_j - \epsilon_F) - \theta(t'-t)\theta(\epsilon_F - \epsilon_j)] \end{aligned} \tag{32}$$

for $t > t'$ the propagation involves energy states above the Fermi energy (particle excitations), for $t < t'$ it involves states below the Fermi energy (hole excitations).