Lection 3-4: Green's functions

• Now we have all necessary tools: second quantization and Wick's theorem to intoduce Green's functions. (1)

Recall the propagation function of one-body theory

$$G_0 = \langle x,t | x',t' \rangle = \langle 0 | \hat{\psi}(x,t)\, \hat{\psi}^{+}(x',t') | 0 \rangle$$

where the field operators are in Heisenberg representation

$$\hat{\psi}(x,t) = e^{i\hat{H}t}\, \hat{\psi}(x)\, e^{-i\hat{H}t}$$ where $\hat{H}$ is a stationary Hamilton

and $|0\rangle$ is a vaccuum state with no particles.

Now we can generalize this definition to the case of a many-particle system

$$G \sim \langle state | \hat{\psi}(\bar{r},t)\, \hat{\psi}^{+}(r',t') | state \rangle \qquad (*)$$

where $|state\rangle$ designates some state of a many-particle system.

The meaning of this definition is that we add a one additional particle to our system, see how the stat evolves till the time t and then remove the particle and project on the initial state

Also to get rid of the unnecessary microscopic details whe should average Eq. (*) over all occupied states of our system

The averaging is done like usually in statistical physics

$$\langle \hat{A} \rangle = Tr\,(\hat{\rho}\,\hat{A}) \quad \text{where} \quad \hat{\rho} = \exp\left(\beta(\Omega + \mu N - \hat{H})\right)$$

is statistical operator

μ = chemical potential, $\beta = 1/T$

We consider grand caninical ensemble where μ is fixed and

$\Omega = F - \mu N$ is a thermodynamic potential

Since Hamiltonian always commutes with particle number

$$[\hat{H}, \hat{N}] = 0$$

it is convenient to introdeice new Hamiltonian

$$H' = H - \mu N$$

Furthermore the expression (*) should be modified to consider the processes where the particle is removed from the system and then added back at time t. $G \sim \langle \hat{\psi}(t)\hat{\psi}^{+}(t') \rangle \pm \langle \hat{\psi}^{+}(t') \psi(t) \rangle$

For this purpose we should introdeice time-ordered product

Time-ordered product is defined as

$$T\, A(t_1) B(t_2) = \begin{cases} A(t_1) B(t_2) & t_1 > t_2 \\ \mp B(t_2) A(t_1) & t_1 < t_2 \end{cases}$$

where $-$ Fermions
$+$ Bosons

Finally we come to the definition of <u>the causal G function</u>

$$G(r_1 t_1, r_2 t_2) = -i\, Tr\left[\hat{\rho}\, T\, \hat{\psi}(r_1, t_1)\, \hat{\psi}^+(r_2, t_2)\right]$$

This definition is general and works for any temperature. Howeve at $T=0$ the average reduces to the ground state

$$Tr\,(\hat{\rho}\, T \psi_1 \psi_2^+) = \sum_{n,m} \langle n | \exp(\beta(\Omega - H)) | m \rangle \langle m | T \psi_1 \psi_2^+ | n \rangle \cdot \frac{1}{\langle n|n\rangle \langle m|m\rangle}$$

$$= \exp(\beta\Omega) \sum_n \exp(-\beta(E_n - \mu N_n)) \langle n | T \psi_1 \psi_2^+ | n \rangle \frac{1}{\langle n|n\rangle}$$

$$= \frac{\sum_n \exp(-\beta(E_n - \mu N_n)) \langle n | T \psi_1 \psi_2^+ | n \rangle}{\langle n|n\rangle \sum_n \exp(-\beta(E_n - \mu N_n))} \xrightarrow[\beta \to \infty]{} \frac{\langle 0 | T \psi_1 \psi_2^+ | 0 \rangle}{\langle 0|0\rangle}$$

Here $|0\rangle$ is the ground state which has minimal energy $E_0 - \mu N_0$
$|0\rangle$ is in the Heisenberg representation so it is time-independent

In a homogeneous and isotropic system in stationary state
GF depends only on relative coordinate and time

Homogeneous : $G(r_1 t_1, r_2 t_2) = G(r_1 - r_2, t_1 - t_2)$
Stationary

We can add spin coordinates as well $\quad \hat{\psi} = \hat{\psi}_\alpha(r, t) \quad G = G_{\alpha\beta}(r_1 t_1, r_2 t_2)$

without magnetic order $\quad G_{\alpha\beta} = G\, \delta_{\alpha\beta}$

Unperturbed Green's functions of Fermions

It is instructive to calculate GF of free fermions and phonons starting from definition.

We consider zero-temperature case

$$G^0(r,t) = -i\langle 0|T\,\psi(r,t)\,\psi^+(0,0)\,|0\rangle$$

In momentum representation

$$\psi(r,t) = \frac{1}{\sqrt{V}}\sum_k a_k \exp(ikr - i(\varepsilon_k-\mu)t) \qquad \text{where } \varepsilon_k = \frac{\hbar^2k^2}{2m}$$

Taking into account that in the ground state $\langle a_k^+ a_{k'}\rangle_0 = \theta(\mu-\varepsilon_k)\delta_{kk'}$

we get

$$\langle T\psi(r,t)\psi^+(0,0)\rangle_0 = \theta(t)\langle\psi(r,t)\psi^+(0,0)\rangle_0 - \theta(-t)\langle\psi^+(0,0)\psi(r,t)\rangle =$$

$$= \frac{1}{V}\sum_{k,k'}\left[\theta(t)\,a_k a_{k'}^+ - \theta(-t)\,a_{k'}^+ a_k\right]\exp(ikr - i(\varepsilon_k-\mu)t) =$$

$$= \frac{1}{V}\sum_k\left[\theta(t)(1-\theta(\mu-\varepsilon_k)) - \theta(-t)\,\theta(\mu-\varepsilon_k)\right]\exp(ikr - i(\varepsilon_k-\mu)t)$$

Fourier transform $G(k,\omega) = \int \exp(-ikr + i\omega t)\,G(r,t)\,d^3r\,dt$

We use $\int e^{i\omega t}\theta(\pm t)\,dt = \frac{\pm i}{\omega \pm i0}$

Hence

$$G(k,\omega) = -i\left[\frac{+i}{\omega+i0}(1-\theta(\mu-\varepsilon_k)) + \frac{i}{\omega-i0}\theta(\mu-\varepsilon_k)\right] = \frac{1}{\omega-(\varepsilon_k-\mu)+i0\,\mathrm{sgn}(\varepsilon_k-\mu)}$$

$$= \frac{1}{\omega-(\varepsilon_k-\mu)+i0\,\mathrm{sgn}\,\omega}$$

The infinitizemal term in the denominator indicates in what half-plane of complex frequency the corresponding integral will converge, exactli like for one-particle propagator. The difference is that we have both $\theta(t)$ and $\theta(-t)$ in the causal GF.

Unperturbed Green's functions : phonons

$$D(r,t) = -i \langle T \varphi(r,t)\, \varphi(0,0) \rangle_0$$

Phononic field is Hermitian $\varphi(r,t) = \varphi^+(r,t)$

$$\varphi(r,t) = \frac{1}{\sqrt{V}} \sum_k \sqrt{\frac{\omega_k}{2}} \left[\hat{b}_k e^{i(kr-\omega_k t)} + \hat{b}_k^+ e^{-i(kr-\omega_k t)} \right]$$

where $\hat{b}, \hat{b}^+$ are bosonic operators

In the ground state $\langle b_k b_{k'}^+ \rangle_0 = \delta_{kk'}$ $\langle b_k^+ b_{k'} \rangle_0 = 0$

$$\langle T\, \varphi(r,t) \varphi \rangle_0 = \Theta(t) \langle \varphi(r,t)\, \varphi(0,0) \rangle + \Theta(-t) \langle \varphi(0,0)\, \varphi(r,t) \rangle_0 =$$

$$= \frac{\sqrt{\omega_k \omega_{k'}}}{2V} \sum_{kk'} \left[\Theta(t) \langle (b_k e^{i\alpha_k} + b_k^+ e^{-i\alpha_k})(b_{k'} + b_{k'}^+) \rangle_0 + \Theta(-t) \langle (b_{k'} + b_{k'}^+)(b_k e^{i\alpha_k} + b_k^+ e^{-i\alpha_k}) \rangle \right]$$

$$= \frac{\sqrt{\omega_k \omega_{k'}}}{2V} \sum_{kk'} \Theta(t) \langle b_k b_{k'}^+ \rangle_0 e^{i\alpha_k} + \Theta(-t) \langle b_{k'} b_k^+ \rangle e^{-i\alpha_k} = \frac{1}{2V} \sum_k \left(\Theta(t) e^{i\alpha_k} + \Theta(-t) e^{-i\alpha_k} \right) \omega_k =$$

Fourier transform:

$$D(\omega,k) = \frac{-i}{2V} \int \sum_{k'} \left(\Theta(t) e^{i(k'r-\omega_{k'} t)} + \Theta(-t) e^{-ik'r + i\omega_{k'} t} \right) \omega_{k'} e^{i\omega t} e^{-ikr} d^3r\, dt =$$

$$= -\frac{i}{2} \left[\frac{i\omega_k}{\omega - \omega_k + i0} - \frac{i\omega_k}{\omega + \omega_k - i0} \right] = \frac{1}{2} \frac{\omega_k(\omega + \omega_k) - \omega_k(\omega - \omega_k)}{(\omega - \omega_k + i0)(\omega + \omega_k - i0)} = \frac{\omega_k^2}{\omega^2 - \omega_k^2 + i0}$$

The unperturbed GF is a GF in the mathematical sense.

For fermions.
$$\left(i\hbar \frac{\partial}{\partial t_1} - \hat{H}(r_1) \right) G^0(r_1 t_1, r_2 t_2) = \delta(r_1 - r_2)\, \delta(t_1 - t_2)$$

Symbolically this can be written

$$(G^0)^{-1}(1)\, G^0(1,2) = \hat{I}$$

Analytic properties of GF

We have seen that causal GF is non-analytic

Some important properties of GF can be obtained from general physical considerations.
Specifically we will derive the Köllen-Lehman representation for GF which determines its analytic properties in complex ω plane

(5)

Let's consider homogeneous and stationary state. Then we can determine time and spatial dependencies of matrix elem. of Heisenberg operators

$$\psi(t,r) = \exp(iH't)\,\psi(r)\exp(-iH't) \qquad H' = H - \mu t$$

Indeed $\langle n|\psi(t,r)|m\rangle = e^{i\omega_{nm}t}\langle n|\psi(r)|m\rangle$

where $\omega_{nm} = E_n - E_m - \mu(N_n - N_m) = E_n(N) - E_m(N+1) + \mu$

Coordinate dependence: $\psi(r) = e^{i\hat{p}r}\,\psi(0)\,e^{-i\hat{p}r}$ where $\hat{p}$ is total moment

Then:

$$\langle n|\psi(t,r)|m\rangle = e^{i(\omega_{nm}t - ik_{nm}r)}\langle n|\psi(0,0)|m\rangle$$

$$\langle n|\psi^+|m\rangle = \langle m|\psi|n\rangle^* \qquad \text{where } k_{nm} = P_n - P_m$$

Now we can calculate GF

$$\langle T\psi(r,t)\psi^+(0,0)\rangle_0 = \Theta(t)\langle\psi(r,t)\psi^+(0,0)\rangle \mp \Theta(-t)\langle\psi^+(0,0)\psi(r,t)\rangle =$$

$$= \Theta(t)\langle 0|\psi(r,t)|n\rangle\langle n|\psi^+(0,0)|0\rangle \mp \Theta(-t)\langle 0|\psi^+(0,0)|n\rangle\langle n|\psi(r,t)|0\rangle =$$

$$= \Theta(t)\exp(i\omega_{0n}t - ik_{0n}r)\,|\langle 0|\psi(0,0)|n\rangle|^2 \mp \Theta(-t)\exp(+i\omega_{n0}t - ik_{n0}r)\,|\langle n|\psi(0,0)|0\rangle|^2$$

where $\boxed{\begin{aligned}\omega_{0n} &= E_0(N) - E_n(N+1) + \mu\\ \omega_{n0} &= E_n(N-1) - E_0(N) + \mu\end{aligned}}$

Fourier transform

$$G(k,\omega) = \iint G(r,t)\,e^{i\omega t - ikr}\,d^3r\,dt =$$

$$-i(2\pi)^3\left[\frac{i\delta(k-k_{0n})}{\omega+\omega_{0n}+i0}|\langle 0|\hat{\psi}(0)|n\rangle|^2 \pm \frac{i\delta(k+k_{n0})}{\omega+\omega_{n0}-i0}|\langle n|\psi(0)|0\rangle|^2\right] =$$

$$= (2\pi)^3\sum_n\left[\frac{\delta(k-k_n)\,A_n}{\omega+\mu+E_0(N)-E_n(N+1)+i0} \pm \frac{\delta(k+k_n)\,B_n}{\omega+\mu+E_n(N-1)-E_0(N)-i0}\right]$$

where $k_n = k_{0n} = -k_{n0}$ since $k_0 = 0$

we can introduce excitation energies

Add particle: $\varepsilon_n^{(+)} = E_m(N+1) - E_0(N) = E_n(N+1) - E_0(N+1) + \mu > \mu$

Remove particle: $\varepsilon_n^{(-)} = -E_n(N-1) + E_0(N) = E_0(N-1) - E_n(N-1) + \mu < \mu$

Indeed $E_0(N+1) - E_0(N) = \dfrac{\partial E_0}{\partial N} = \mu$

We will discuss physical sence of $\varepsilon_n^{(\pm)}$ below

Thus we obtain finally

$$G(k,\omega) = (2\pi)^3 \sum_n \left[\frac{A_n \delta(k-k_n)}{\omega+\mu-\varepsilon_n^{(+)}+i0} \pm \frac{B_n \delta(k-k_n)}{\omega+\mu-\varepsilon_n^{(-)}-i0} \right] \quad (*)$$

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Let us employ the integral relation

$$\int \frac{f(x)dx}{x\pm i0} = P\int \frac{f(x)}{x}dx \mp i\pi f(0) \qquad \text{where } P\left(\frac{1}{x}\right) = \text{principal value}$$

Poles of G

Then $$\operatorname{Re} G = (2\pi)^3 \sum_n P\left[\frac{A_n \delta(k-k_n)}{\omega+\mu-\varepsilon_n^{+}} + \frac{B_n \delta(k-k_n)}{\omega+\mu-\varepsilon_n^{(-)}} \right]$$

$$\operatorname{Im} G = \begin{cases} -(2\pi)^3\pi \sum_n A_n \delta(k-k_n)\,\delta(\omega+\mu-\varepsilon_n^{(+)}) & \omega>0 \\ \pm(2\pi)^3\pi \sum_n B_n \delta(k-k_n)\,\delta(\omega+\mu-\varepsilon_n^{(-)}) & \omega<0 \end{cases}$$

so that $\operatorname{sign} \operatorname{Im} G(\omega,k) = -\operatorname{sign}\omega$ for Fermi system

$\operatorname{sign} \operatorname{Im} G(\omega,k) = -1$ for Bose

Asymptotic behaviour $G(\omega) \sim 1/\omega$ at large ω.

Indeed from (*) we get

$$G = (2\pi)^3 \frac{1}{\omega} \sum_n A_n \delta(k-k_n) \pm B_n \delta(k-k_n) =$$

$$= \frac{(2\pi)^3}{\omega} \sum |\langle 0|\psi|n\rangle|^2 \delta(k-k_n) \pm |\langle n|\psi|0\rangle|^2 \delta(k-k_n) = \frac{1}{\omega}\int e^{ikx}\left(\psi(t,x_1)\psi^+(t,x_2) \pm \psi^+(t,x_2)\psi(t,x_1)\right)$$

$$= \frac{1}{\omega}$$

<u>Quasiparticle excitations</u>

The main property of GF in momentum space which we can derive from KL representation is that it has poles at $\omega = \varepsilon_m - \mu$ where ε_m are discrete excitation energies. In the thermodynamic limit $N\to\infty$ some poles disappear. That is if there are many degenerate states with different energies ε_n but the same $k_n = k$ the poles will be eliminated.

However if there is an unambiguous dispersion relation

$$\varepsilon_n = \varepsilon_n(k)$$

the poles will survive. Qualitatively it means that momentum and energy are carried by quasipartice

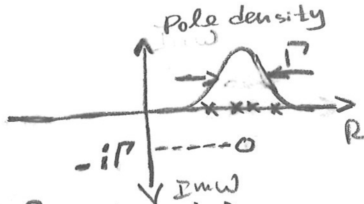
$$G^{-1}(\omega,k) \sim \omega+\mu-\varepsilon_n(k).$$

Hence the equation $G^{-1}(\varepsilon-\mu, k) = 0$ determines <u>quasiparticle spectrum</u>

Bonch-Bruevich

1955

On the other hand, those poles which survive can obtain a finite shift to complex plane.



If we sum up contributions from many poles on the real axis concentrated near some frequency ω_0 then effectively we get the result as if from the single pole but shifted to imaginary plane.

$$\int_{-\infty}^{\infty} e^{-i\omega t}\,\frac{d\omega}{(\omega-\omega_0)^2+\Gamma^2} = -\pi i\, e^{-i\omega_0 t-\Gamma t} = -\frac{k}{2}\int_{-\infty}^{\infty} e^{-i\omega t}\,\frac{d\omega}{\omega-\omega_0+i\Gamma}$$

Therefore the quasiparticle energy is complex

$$\varepsilon = \varepsilon(k) - \mu + i\Gamma \qquad (7)$$

According to genelal quantum mechanics rules the complex energy means finite quasiparticle lifetime $\tau \sim 1/|\mathrm{Im}\,\varepsilon|$

The quasiparticle meacture is meaningfull while lifetime is long

$$|\varepsilon-\mu| \gg |\mathrm{Im}\,\varepsilon|$$

Retarded and advanced GF

Suppose that we know there is a quasiparticle with certain energy and lifetime so that there is a pole

$$\omega = \Omega - i\Gamma$$

Let us calculate time dependense of the GF at $t>0$

$$G(t,k) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, e^{-i\omega t}\, G(\omega,k)$$

We can not just take a residue because $G(\omega,k)$ can have other singularities. Steel the calculation is possible in quite a general form.

In order to do this let us introduce retarded and advanced GF which have a remarkable property: they are analytic continuation of the causal GF to the complex plane.

$$G^R(r_1t_1,r_2t_2) = -i\left\langle \psi(r_1,t_1)\psi^+(r_2t_2) \pm \psi^+(r_2t_2)\psi(r_1,t_1)\right\rangle \theta(t_1-t_2)$$

$$G^A(r_1t_1,r_2t_2) = +i\left\langle \psi(r_1t_1)\psi^+(r_2t_2) \pm \psi^+(r_2t_2)\psi(r_1,t_1)\right\rangle \theta(t_2-t_1)$$

The definition is chosen in such a way that $G^R=0$ for $t_1<t_2$ and G^A for $t_1>t_2$. At $t_1=t_2$ they both have a discontinuity same as G so that $\left[G^{R,A}\right]_{t_1=t_2} = -i\delta(r_1-r_2)$

The Källén-Lehmann representation for $G^{R,A}$ can be obtained analogously to G

$$G^R(k,\omega) = (2\pi)^3 \sum_n \frac{A_n \delta(k-k_n)}{\omega - \varepsilon_n^{(+)} + \mu + i0} \pm \frac{B_n \delta(k+k_n)}{\omega - \varepsilon_n^{(-)} + \mu + i0}$$

$$G^A(k,\omega) = (2\pi)^3 \sum_n \frac{A_n \delta(k-k_n)}{\omega - \varepsilon_n^{(+)} + \mu - i0} \pm \frac{B_n \delta(k+k_n)}{\omega - \varepsilon_n^{(-)} + \mu - i0}$$

One can see that G^R (G^A) is analytic in the upper (lower) ω-half plane

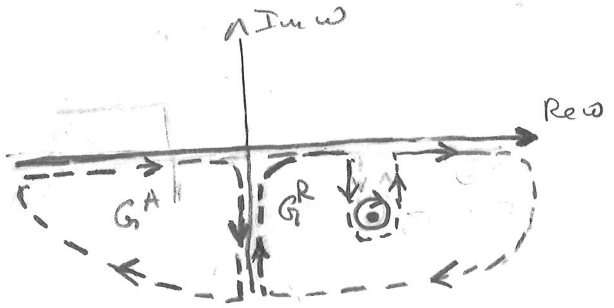
On the other hand we see that on the real axis

$$\mathrm{Re}\, G^R = \mathrm{Re}\, G^A = \mathrm{Re}\, G$$

$$\mathrm{Im}\, G^R = \mathrm{Im}\, G \qquad \omega > 0$$

$$\mathrm{Im}\, G^A = \mathrm{Im}\, G \qquad \omega < 0$$

$$G^R = (G^A)^*$$



Let us now calculate the time dependence

$$\int_{-\infty}^{\infty} G(\omega,k)\, e^{-i\omega t} \frac{d\omega}{2\pi} = \int_{-\infty}^{0} G^A(\omega,k)\, e^{-i\omega t} \frac{d\omega}{2\pi} + \int_0^{\infty} G^R(\omega,k) e^{-i\omega t} \frac{d\omega}{2\pi} =$$

$$= \int_{-i\infty}^{0} \frac{d\omega}{2\pi} e^{-i\omega t} (G^A - G^R) + \int_C \frac{d\omega}{2\pi} e^{-i\omega t} G^R = -iA\, e^{-i\Omega t} e^{-\Gamma t} + \int_{-i\infty}^{0} \frac{d\omega}{2\pi} e^{-i\omega t} (G^A - G^R) =$$

$$= -iA\, e^{-i\Omega t - \Gamma t} + \frac{2i\Gamma A}{2\pi} \int_{-\infty}^{0} \frac{e^{-i\omega t}}{(\omega-\Omega)^2 + \Gamma^2} d\omega =$$

$$= -iA\, e^{-i\omega t - \Gamma t} + \frac{\Gamma A}{\pi t} \frac{e^{-i\omega t}}{\Omega^2}$$

Consider simple model

$$G^R(\mathrm{Re}\,\omega > 0) = \frac{A}{\omega - \Omega + i\Gamma}$$

$$G^A - G^R = \frac{2i\Gamma A}{(\omega-\Omega)^2 + \Gamma^2}$$

$$G^A(\mathrm{Re}\,\omega < 0) = \frac{A}{\omega - \Omega - i\Gamma}$$

The second term is smaller if $\Gamma \ll \Omega$

In this case the state with additional particle propagates like an approximate eigenstate $\hbar\Omega$

Kramers-Kronig relations

From Källén-Lehmann representation it immediately follows that

$$\mathrm{Re}\, G^{R,A} = \pm P \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\mathrm{Im}\, G^{R,A}}{\omega' - \omega}$$

No poles in upper plane

$$0 = \int_{-\infty}^{\infty} \frac{G^R(\omega')}{\omega - \omega' + i0} d\omega' = P \int \frac{G^R}{\omega - \omega'} d\omega + i\pi G^R(\omega) = 0$$

These relations hold for any functions which are analytic at upper (lower) half-plane. The physical reason for this is causality principle.

Green's functions and observables.

The way of expressing observables - that is average values of quantum mechanical operators directly follows from the definition of the GF.

$$G_{\alpha\beta} = -i \langle 0 | T\, \psi_\alpha(r,t')\, \psi^+_\beta(r,t) | 0 \rangle$$

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1) Particle density

$$n(r) = \langle \psi^+_\alpha(r)\, \psi_\alpha(r) \rangle = \overset{\text{Fermi}}{\mp}\, i\, G_{\alpha\alpha}(r, t-0, r, t)$$

Then for fermion homogeneous system $\quad n(r) = 2\, \mathrm{Im}\, G(r, t=-0)$

2) Current $\quad \hat{j} = \frac{ie}{2m} \sum_\alpha \partial^*_r \psi^+_\alpha(r)\, \psi_\alpha(r) - \psi^+_\alpha(r)\, \partial_r \psi_\alpha(r) \qquad$ where $\partial_r = \nabla + \frac{ie}{\hbar c} A$

Hence

$$j = \frac{ie}{2m} \lim_{r \to r'} (\nabla_r - \nabla_{r'}) \langle \psi^+_\alpha(r)\, \psi_\alpha(r') \rangle + \frac{e^2}{m\hbar c} A \langle \psi^+_\alpha(r)\, \psi_\alpha(r) \rangle =$$

$$= \frac{ie}{2m} \sum_\alpha \lim_{\substack{t \to -0 \\ r \to r'}} (\nabla_{r'} - \nabla_r) \left(\mp i\, G_{\alpha\alpha}(r', t, r, 0) \right) + \frac{e^2}{m\hbar c} \vec{A}\, n(r)$$

$$= \mp \frac{e}{2m} \lim_{\substack{r \to r' \\ t \to -0}} (\nabla_r - \nabla_{r'})\, G_{\alpha\alpha}(r, t, r', 0) - \frac{e^2}{m\hbar c} \vec{A}\, n$$

In principle at $T=0$ $G^{R,A}$ are useless since we can calculate G causal directly. But at finite T they are the only way to develop perturbation theory is to use analytical continuations of $G^{R,A}$