- using perturbation theory or numerical methods
- singular - requires $\eta \to 0^+$ in def^n
- fortunately it can be related exactly to Matsubara (imaginary time) GF which (by analytic continuation) is much easier to calculate - many types of calculation [pert. theory, QMC] calculate M. GF first [but not all - lately real time DMRG methods introduced]
- let τ be "imaginary time" and define operators at imaginary time τ as

$$\mathcal{O}(\tau) \equiv e^{H\tau}\, \mathcal{O}\, e^{-H\tau}$$

- like def^n of Heis. pic. ops with $t \to -i\tau$

[$\mathcal{O}$ here is $\mathcal{O}_\tau = \mathcal{O}_H(t=0)$]

- this is convenient because finite T Green's functions in real time involve

$$\mathrm{tr}\left(e^{-\beta H}\,\mathcal{O}(t)\,\mathcal{O}(0)\right)$$
$$= \mathrm{tr}\left(e^{-\beta H}\;e^{iHt}\mathcal{O}\,e^{-iHt}\mathcal{O}\right)$$

- H occurs in 2 quite different ways - t-evolution & Boltzmann factor
- first with i, second with no i
- imaginary time GF involve

$$\mathrm{tr}\left(e^{-\beta H}\;e^{\tau H}\mathcal{O}\,e^{-\tau H}\mathcal{O}\right)$$
$$= \mathrm{tr}\left(e^{-(\beta-\tau)H}\mathcal{O}\,e^{-\tau H}\mathcal{O}\right)$$

- no i's in exponents
- one other important feature: Matsubara GF is <u>time</u> <u>ordered</u> - time-ordering can be defined for real or imaginary time

$$T\left[A(\tau_1)\,B(\tau_2)\right] = A(\tau_1)\,B(\tau_2), \qquad \tau_1 > \tau_2$$
$$= B(\tau_2)\,A(\tau_1), \qquad \tau_2 > \tau_1$$

<u>latest</u> on <u>left</u>

same defn for real or imaginary time

$T[A_1(\tau_1) \cdots A_n(\tau_n)]$ permutes operators to order

latest --- earliest

- this was for bosonic ops
- for fermionic ops $C_{\vec{p}\sigma}$, $C^{\dagger}_{\vec{p}'\sigma'}$, we add minus signs to defn

$T[C_{\vec{p}_1\sigma_1}(\tau_1), C^{\dagger}_{\vec{p}_2\sigma_2}(\tau_2)]$

$= C_{\vec{p}_1\sigma_1}(\tau_1) C^{\dagger}_{\vec{p}_2\sigma_2}(\tau_2), \quad \tau_1 > \tau_2$

$= - C^{\dagger}_{\vec{p}_2\sigma_2}(\tau_2) C_{\vec{p}_1\sigma_1}(\tau_1), \quad \tau_2 > \tau_1$

- with this defn, T ordering has no effect on "independent" ops which anti-commute - eg $C_{\uparrow}$, $C^{\dagger}_{\downarrow}$ [for most Hamiltonians] or $C_{\vec{p}\sigma}$, $C_{\vec{p}'\sigma'}$

- ~~Matsubara GF~~ for

Matsubara GF for operator $\mathcal{O}$, $\mathcal{O}^+$ is defined as.

$$\mathcal{G}(\tau_1, \tau_2) = - T \langle \mathcal{O}(\tau_1) \mathcal{O}^+(\tau_2) \rangle$$

$$\equiv -\frac{1}{Z} tr \left[e^{-\beta H} T \left(\mathcal{O}(\tau_1) \mathcal{O}^+(\tau_2) \right) \right]$$

$$= -\frac{1}{Z} tr \left[e^{-(\beta - \tau_1)H} \mathcal{O} e^{-\beta(\tau_1 - \tau_2)} \mathcal{O}^+ e^{-\beta \tau_2} \right] \quad \tau_1 > \tau_2$$

$$= \mp \frac{1}{Z} tr \left[e^{-(\beta - \tau_2)H} \mathcal{O}^+ e^{-\beta(\tau_2 - \tau_1)} \mathcal{O} e^{-\beta \tau_1} \right], \quad \tau_2 > \tau_1$$

- a function of $\tau_1 - \tau_2$ only using

$$Tr(ABC) = Tr(CAB)$$

$$e^{-\beta \tau_2} e^{-(\beta + \tau_1)H} = e^{-(\beta - \tau_1 + \tau_2)H} \quad etc.$$

$\mp$ - boson
 - fermion

- we restrict ~~τ_i to~~

$$\mathcal{G} = \mathcal{G}(\tau)$$

- we restrict τ to $|\tau| < \beta$

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so factor $e^{-(\beta \pm \tau)H}$ involve negative numbers multiplying H in exponent - this guarantees good behavior when we insert complete set of states - high energy states suppressed

- in fact, $\mathcal{G}(\tau+\beta) = \pm \mathcal{G}(\tau)$ [B or F]

assume $-\beta < \tau < 0$

$$\mathcal{G}(\tau) = -\frac{1}{Z} tr\left[e^{-\beta H} a^{+} e^{H\tau} a e^{-\tau H}\right]$$

(t - ordered)

$$= -\frac{1}{Z} tr\left[e^{-(\beta+\tau)H} a^{+} e^{H\tau} a\right]$$

$$= -\frac{1}{Z} tr\left[e^{H\tau} a e^{-(\beta+\tau)H} a^{+}\right]$$

$$= -\frac{1}{Z} tr\left[e^{-\beta H} e^{(\tau+\beta)H} a e^{-(\tau+\beta)H} a^{+}\right]$$

$$= -\frac{1}{Z} tr\left[e^{-\beta H} a(\tau+\beta) a^{+}(0)\right]$$

$\tau+\beta > 0$ by assumption

so this $= \pm \mathcal{G}(\tau+\beta)$ $\begin{matrix} B \\ F \end{matrix}$

$\mathcal{G}(\tau)$ is a periodic [anti-periodic] func. with period β]

- simplifies Fourier transforms

$$\mathcal{G}(i\omega_n) = \int_0^\beta d\tau\, \mathcal{G}(\tau)\, e^{i\tau\omega_n}$$

where $\omega_n = \frac{2\pi n}{\beta}$ — B

$\frac{2\pi}{\beta}(n+\frac{1}{2})$ — F

- integral over $0<\tau<\beta$ only — 1 period

- slightly funny notation $\mathcal{G}(i\omega_n)$ not $\mathcal{G}(\omega_n)$ (Mahan)

$$\mathcal{G}(\tau) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-i\omega_n\tau}\,\mathcal{G}(\omega_n)$$

$$\mathcal{G}(i\omega_n) = -e^{\beta\Omega}\int_0^\beta d\tau\, \mathrm{tr}\left[e^{-(\beta-\tau)H} a\, e^{-\tau H} a^+\right] e^{i\tau\omega_n}$$

(since $\tau>0$, latest on left)

- Now consider spectral resolution to establish connection with G_{ret}:

$$\mathcal{G}(i\omega_n) = -e^{\beta\Omega}\sum_{pm}\int_0^\beta d\tau \, (\mp) \langle p|e^{-(\beta-\tau)H}U|m\rangle$$

$$\langle m|e^{-\tau H}U^{+}|p\rangle \, e^{i\tau\omega_n}$$

$$= -e^{\beta\Omega}\sum_{pm} |\langle p|U|m\rangle|^2 \int_0^\beta d\tau \, e^{-\beta E_p - \tau(E_m - E_p) + i\tau\omega_n}$$

$$\int_0^\beta d\tau \, e^{\tau(i\omega_n + E_p - E_m)}$$

$$= \frac{1}{i\omega_n + E_p - E_m}\left[e^{i\omega_n\beta}e^{\beta(E_p-E_n)} - 1\right]$$

$$e^{i\omega_n\beta} = \begin{array}{cc} 1 & B \\ -1 & F \end{array}$$

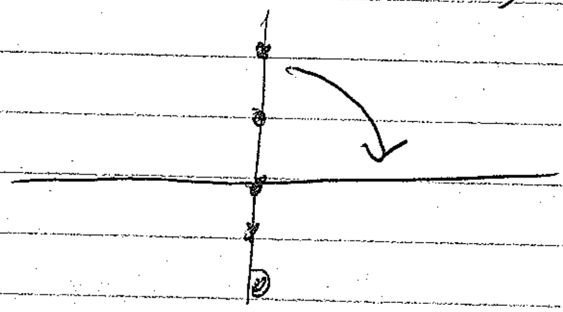
$$\Rightarrow \int_0^\beta d\tau \, e^{\tau(i\omega_n + E_p - E_m)} = \begin{array}{ll} e^{\beta(E_p-E_m)} - 1 & B \\ = -\left[e^{\beta(E_p-E_m)} + 1\right] & F \end{array}$$

(given in terms of Bose or Fermi dist. fnc.)

$$\mathcal{G}(i\omega_n) = -e^{\beta\Omega}\sum_{p,m} \frac{|\langle p|U|m\rangle|^2\left[\pm e^{-\beta E_m} - e^{-\beta E_p}\right]}{i\omega_n + E_p - E_m} \quad \left[\begin{array}{c} B \\ F \end{array}\right]$$

- if we let $i\omega_n \to \omega + i\eta$ ($\eta \to 0^+$) this becomes identical to retarded GF in both boson fermion cases

- so a common procedure is to first calculate $G(i\omega_n)$ then attempt to do analytic continuation to real [ω ~~frequen~~ ~~axis~~ axis (from above)



(β-case)

- it is normally straightforward to perform analytic continuation order by order in perturbation theory [simple fncs of $i\omega_n$]
- often difficult numerically
- in fact, analytic continuation from a discrete set of points to entire complex plane [e in particular to $\omega+i\eta$] is not unique
- we chose continuation that is analytic in

upper half-plane - generally fixes it uniquely

- appropriate sum

$$G_{ret}(\omega) = \lim_{\eta \to 0^+} \int_0^\infty dt\, e^{i(\omega + i\eta)t}\, G_{ret}(t)$$

- expect integral to converge if ω has imaginary part ≥ 0, assuming $G_{ret}(t)$ doesn't blow up at large t

- $G_{ret}(\omega)$ generally has singularities on real axis and lower half-plane

<u>Free fermion GF</u>

~~$\mathcal{G}^{(0)}(\vec{p}\,\tau) = - T \langle C_{\vec{p}\sigma}(\tau)\; C_{\vec{p}}$~~

$$\mathcal{G}^{(0)}(\vec{p}, \tau) = - T \langle C_{\vec{p}}(\tau)\, C_{\vec{p}}^{+}(0) \rangle$$

NB $T \langle C_{\vec{p}\sigma}\, C^{+}_{\vec{p}'\sigma'} \rangle \propto \delta_{\vec{p},\vec{p}'}\, \delta_{\sigma\sigma'}$

why? $\langle n | C_{\vec{p}\sigma}\, C_{\vec{p}'\sigma'}^{+} | n \rangle = 0$ for any eigenstate $|n\rangle$ unless $(\vec{p} = \vec{p}')$ and $(\sigma = \sigma')$

since $|n\rangle$ is an eigenstate of $\hat{n}_{\vec{p}\sigma}$

- so ~~supp~~ focus on diagonal part and suppress σ index

$$\mathcal{G}^{(0)}(\vec{p},\tau) = -\langle e^{\tau H} c_{\vec{p}}\, e^{-\tau H} c_{\vec{p}}^{\dagger} \rangle, \quad \tau > 0$$

$$= \langle c_{\vec{p}}^{\dagger}\, e^{\tau H} c_{\vec{p}}\, e^{-\tau H} \rangle, \quad \tau < 0$$

- note that acting on any energy eigenstate $|n\rangle$; $c_{\vec{p}}$ ~~lowers~~ changes energy by $-\epsilon_{\vec{p}}$

$$\Rightarrow e^{\tau H} c_{\vec{p}}\, e^{-\tau H} = e^{-\tau \epsilon_{\vec{p}}} c_{\vec{p}}$$

$$\left[= e^{\tau(E_n - \epsilon_{\vec{p}})} c_{\vec{p}}\, e^{-\tau E_n} \right]$$

$$\mathcal{G}^{(0)}(\vec{p},\tau) = -e^{-\tau \epsilon_{\vec{p}}} \langle c_{\vec{p}} c_{\vec{p}}^{\dagger} \rangle, \quad \tau > 0$$

$$= e^{-\tau \epsilon_{\vec{p}}} \langle c_{\vec{p}}^{\dagger} c_{\vec{p}} \rangle, \quad \tau > 0$$

$$\langle c_{\vec{p}}^{\dagger} c_{\vec{p}} \rangle = n_F(\epsilon_{\vec{p}}) = \frac{1}{e^{\beta \epsilon_{\vec{p}}} + 1}$$

$$\langle c_{\vec{p}} c_{\vec{p}}^{\dagger} \rangle = 1 - n_F \quad \left[\cancel{= \frac{1}{e^{-\beta \epsilon_{\vec{p}}} + 1}} \right]$$

$$\mathcal{G}^{(0)}(\vec{p},\tau) = e^{-\tau \epsilon_{\vec{p}}} \left[n_F(\epsilon_p) - \theta(\tau) \right]$$

where $\theta(\tau) = 1, \; \tau > 0$
$\qquad\qquad = 0, \; \tau < 0$

$\mathcal{G}^{(0)}(\vec{p},\tau)$ is discontinuous at $\tau = 0$

we take this as def^{n} for $|\tau| < \beta$ only

Fourier transform:

$$\mathcal{G}(\vec{p}, \omega_n) = \int_0^\beta d\tau\, e^{i\omega_n \tau} \mathcal{G}(\tau)$$

$$\omega_n = \frac{2\pi}{\beta}(n+\tfrac{1}{2})$$

since $\mathcal{G}(\tau+\beta) = -\mathcal{G}(\tau+\beta)$

NB – can integrate over any interval of period β

in domain $|\tau| < \beta$ and get same result

$$\mathcal{G}(\vec{p}, \omega_n) = [n_F(\epsilon_p) - 1] \int_0^\beta d\tau\, e^{i\omega_n \tau} e^{-\epsilon_p \tau}$$

$$= (n_F - 1) \frac{[e^{i\omega_n\beta} e^{-\epsilon_p \beta} - 1]}{i\omega_n - \epsilon_p}$$

$e^{i\omega_n \beta} = -1$ (why?) $\rightarrow$

$$\mathcal{G}(\vec{p}, \tau) = -\frac{(n_F - 1)[e^{-\beta\epsilon_p} + 1]}{i\omega_n - \epsilon_p} = \frac{1}{i\omega_n - \epsilon_p}$$

– very simple result! – true at finite T

but no T-dependence except in allowed

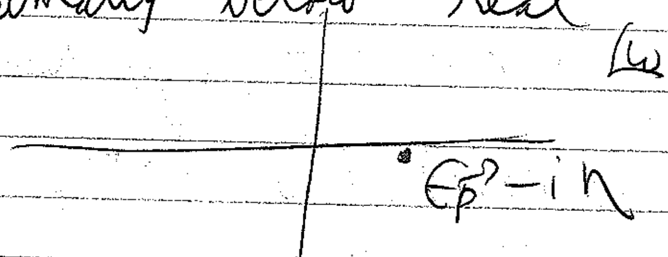
values of $\omega_n = \frac{2\pi}{\beta}(n+\tfrac{1}{2})$

now let $i\omega_n \to \omega + i\eta$ to get

$$G^{(0)}_{ret}(\vec{p},\omega) = \frac{1}{\omega - \epsilon_{\vec{p}} + i\eta}$$

- no T-dependence whatsoever!
- meromorphic fn in complex ω-plane
- only singularity is a pole @ $\omega = \epsilon_{\vec{p}} - i\eta$

(infinitesimally below real axis)

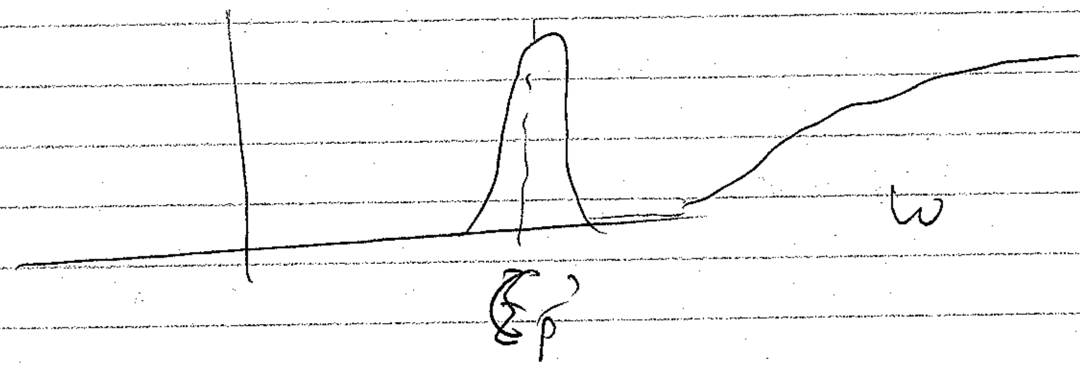


$$\mathrm{Im}\, G^{(0)}_{ret}(\vec{p},\omega) = -\pi\,\delta(\omega - \epsilon_{\vec{p}})$$

- for $\omega > 0$, non-zero for $\epsilon_{\vec{p}} > 0 \Rightarrow \vec{p}$ outside Fermi surface [$p > p_F$ for $p^2/2m$ dispersion]
- comes from C_p^{+} contribution
- for $\omega < 0$, non-zero for $\epsilon_p < 0 \Rightarrow \vec{p}$ inside Fermi surface – $C_{\vec{p}}$ contribution

including interaction, spectral density function takes a non-trivial form

$A(\vec{p},\omega) = -2 \,\mathrm{Im}\, G^{ret}(\vec{p},\omega)$



- single-particle peak can be shifted [renormalization of effective mass], broadened (finite lifetime) & reduced in intensity with some spectral weight occurring at higher energies, corresponding for example to $c_{\vec{p}}^{+}|0\rangle$ creating 2 particles + a hole

- for a clean system [no disorder] Fermi-liquid theory predicts single-particle peak width $\to 0$ at $T, \epsilon_p \to 0$ $\vec{p} \to \vec{p}_f$

- intensity given by a reduction factor Z called "quasi-particle weight"
- for a "non-Fermi liquid" [eg 1D Luttinger liquid] $Z = 0$ – no δ-fn term even at $T, \epsilon_p \to 0$ $p \to p_F$

<u>~~Feynman~~ Path Integrals</u>

- based on correspondance between classical & quantum theory
- start with classical action
- for a single particle moving in a potential $V(\vec{x})$: Lagrangian is defined as

$$L = \frac{m}{2}\dot{\vec{x}}^2 - V(\vec{x}) \quad \left[\dot{\vec{x}} = \frac{d\vec{x}}{dt}\right]$$

$$L = L(\vec{x}, \dot{\vec{x}})$$

$$p_i \equiv \frac{\partial L}{\partial \dot{x}_i} \quad [= \cancel{m\dot{x}^2}\; m\dot{x}_i]$$

"conjugate momentum"

$$H = \sum_i p_i \dot{X}_i - L = \frac{\vec{p}^{\,2}}{2m} + V(\vec{x}) = H(\vec{x}, \vec{p})$$

- these formulas generalize to essentially arbitrary Lagrangians with more co-ordinates
- to quantize theory, we treat X_i, p_i as operators & impose canonical commutation relations: $[X_j, p_k] = i\hbar\, \delta_{jk}$

$[X_j, X_k] = [p_j, p_k] = 0$

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- this generalizes to quantum field theories [in both CMP & HEP]
- for interacting fermions we write action in terms of electron field $\psi_\sigma(\vec{r}, t)$

$$L = i \int d^3\vec{r} \sum_\sigma \psi^\dagger_\sigma(\vec{r}, t) \frac{\partial}{\partial t} \psi_\sigma(\vec{r}, t) - H$$

- conjugate momentum to $\psi_\sigma(\vec{r})$ given by

$$\Pi_\sigma(\vec{r}) = \frac{\delta L}{\delta \dot{\psi}_\sigma(\vec{r})} = i\, \psi_\sigma^\dagger(\vec{r})$$

- canonical quantization obtained by

imposing <u>anti-commutation</u> relations

$$\{ \psi_\sigma(\vec{r}), \Pi_{\sigma'}(\vec{r}') \} = i\delta_{\sigma,\sigma'} \delta^3(\vec{r}-\vec{r}')$$

$$\{ \psi_\sigma(\vec{r}), i\psi^\dagger_{\sigma'}(\vec{r}') \} = i\delta_{\sigma,\sigma'} \delta^3(\vec{r}-\vec{r}')$$

NB - for fermions canonical quantization is modified by imposing <u>anti-commutation</u> relations

also $\{ \psi_\sigma, \psi_{\sigma'} \} = \{ \psi^\dagger_\sigma, \psi^\dagger_{\sigma'} \} = 0$

- the fact that these agree with ones obtained from other considerations shows we wrote correct Lagrangian

action $S = \int dt\, L$

- Feynman path integral in single particle QM

$$ {}_S\langle \vec{X}_f(t_f) | \vec{X}_i(t_i) \rangle_S = {}_H\langle \vec{X}_f | e^{i(t_f - t_i)H} | \vec{X}_i \rangle_H $$

$$\propto \int [d\vec{x}]\, e^{\frac{i}{\hbar} S[\vec{x}(t)]}$$

So here $S[\vec{x}] = \int_{t_i}^{t_f} dt\; L[\vec{x}(t)]$

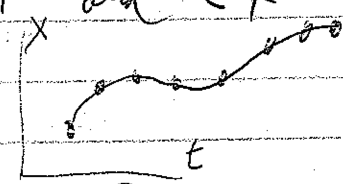
$$= \int_{t_i}^{t_f} dt \left[\tfrac{1}{2} m \dot{\vec{x}}^2 - V(\vec{x}) \right]$$

- we sum over all paths starting at $\vec{x}_i$ at time $t = t_i$, ending at $\vec{x}_f$ at $t = t_f$

$\int [d\vec{x}]$ means sum over all such paths (not just classical ones)

- can be defined by defining a set of times $t_1, t_2, t_3 \ldots t_N$ between t_i and t_f

$$\int [dx(t)] = \prod_{i=1}^{N} \int dx_i$$



where x_i is position at t_i (do it for each component)

- must take limit $N \to \infty$
- see Feynman & Hibbs or Peskin & Schroeder or ...

- called a Feynman path integral - functional integral over all paths $X(t)$

- classical limit is recovered as $\hbar \to 0$ because integral is dominated by classical paths
- follows from "method of steepest descents"
- stationary points $\frac{\delta S}{\delta X_a(t)} = 0$

$$\Rightarrow \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{X}_a}\right) = \frac{\partial L}{\partial X_a}$$

$$m \ddot{X}_a = -\frac{\partial V}{\partial X_a} \quad \text{- E-L equations}$$

- in 2nd quantized theory, fundamental objects are functions of space and time

$\vec{S}_{\vec{R}}(t)$ - spin operator in Heisenberg model or

$\psi_\sigma(\vec{r}, t)$ - electron fields

$$\langle \vec{X}_f | e^{-\beta H} | \vec{X}_i \rangle = \int (\mathcal{D}X)\, e^{S_I}$$

$$S_I = -\int d\tau \left[\frac{m}{2}\left(\frac{d\vec{X}}{d\tau}\right)^2 + V(\vec{X}) \right]$$

(59)

functional integrals are now over these functions of space and time
[time is always a continuous variable although we may discretize it as an approximation space is discrete in lattice models - eg Heisenberg but continuous in continuum models - jellium]

we weight a given "path" - ie field configuration at all space-time points, by classical action

- there is a very profound analogy ~~with~~ between Feynman path integral in quantum many body theory and classical Boltzmann sum ~~is~~ in classical statistical mechanics

- eg - classical Heisenberg model

$$H = J \sum_{\vec{R}, \vec{\delta}} \vec{S}_R \cdot \vec{S}_{R+\delta}$$

$\vec{S}_R$ treated as classical vector of magnitude 1 [or could be magnitude S but absorb that into J]

- classical partition function

$$Z = \prod_{\vec{R}} \int d\vec{S}_R \; e^{-\frac{H[\vec{S}_{R_1}, \ldots \vec{S}_{R_N}]}{T}}$$

- we have an integral of $\vec{S}_R$ over unit sphere at each spatial point $\vec{R}$
- non trivial integrals - lead to phase transitions as functions of T
- to go from classical Boltzmann sum to Feynman path integral we "just" have to extend $\vec{S}_{\vec{R}}$ to $\vec{S}_{\vec{R}}(t)$
- function of time as well as space