Finite temperature many body physics.

* Imaginary time; Schroedinger, Heisenberg, and interaction representations.
* Imaginary time propagator (Green's function)
* periodicity and antiperiodicity
* Matsubara representation
* Feynman rules at finite T.
* Hartree-Fock corrections to the free energy
* Electron in a disordered potential
* Fluctuation-dissipation theorem
* Experimental quantities (spectroscopies).

Finite Temperature Many-Body Physics (Chapter 8)

Zero temp scheme:

$$\langle \phi | T \psi_\alpha(t) \psi^\dagger_\beta(t') | \phi \rangle = \frac{\langle \phi_0 | T \hat{S} \psi_\alpha(t) \psi^\dagger_\beta(t') | \phi_0 \rangle}{\langle \phi_0 | \hat{S} | \phi_0 \rangle}$$

$\phi_0 \rightarrow$ Non interacting

$$\hat{S} = T e^{-i \int_{-\infty}^{\infty} dt'' V(t'')}$$

[Feynman Diagrams to tackle this]

Finite Temp:

Recall from Stat-Mech:

$$\langle \hat{A} \rangle = \frac{\mathrm{Tr}\left[e^{-\beta \hat{H}} \hat{A} \right]}{\mathrm{Tr}\left[e^{-\beta \hat{H}} \right]} = \mathrm{Tr}\left[e^{-\beta(\hat{H} - F)} \hat{A} \right]$$

$\mathrm{Tr}\left[e^{-\beta \hat{H}} \right] \Longrightarrow e^{-\beta F}$

Some similarities in computation of averages:

$$\hat{S} \Leftrightarrow e^{-\beta H} \sim e^{-\int_0^\beta H d\tau} \equiv e^{-i \int_0^{-i\beta} H dt}$$

"imaginary-time evolution"

$t \in [0, -i\beta]$ $\{(-\infty, \infty)$

How does it work:

introduce $\tau \equiv it$

$$\hat{H} |\psi\rangle = -i\partial_t |\psi\rangle \Longrightarrow \hat{H} |\psi\rangle = -\partial_\tau |\psi\rangle$$

$$\Longrightarrow |\psi\rangle = e^{-E\tau} |\psi_0\rangle$$

Need EoM

EoM (by analytic continuation)

$$G_{\alpha\beta}(t,t') = -i \langle \phi | T \psi_\alpha(t) \psi^\dagger_\beta(t') | \phi \rangle \quad \Big\| \quad G_{\alpha\beta}(\tau,\tau') = -\langle\langle T_\tau \psi_\alpha(\tau) \psi^\dagger_\beta(\tau') \rangle\rangle$$

$$\frac{\partial \hat{A}_H}{\partial \tau} = [\hat{H}, \hat{A}_H]; \quad \hat{A}_H = e^{H\tau} A e^{-H\tau}$$

"Zero temperature dynamics / long-time evolution $\overset{\text{analytic}}{\underset{\text{continuation}}{\Longleftrightarrow}}$ Finite T eq. properties"

Imaginary time Propagator (Green's Function)

$$G_{\alpha\beta}(t,t') = -i\langle\phi|T\,\psi_\alpha(t)\psi_\beta^\dagger(t')|\phi\rangle = -i\,\frac{\langle\phi_0|e^{-i\int_{-\infty}^{\infty}V\,dt''}\psi_\alpha(t)\psi_\beta^\dagger(t')|\phi_0\rangle}{\langle\phi_0|e^{-i\int_{-\infty}^{\infty}V\,dt''}|\phi_0\rangle}$$

$\Downarrow$

$$G_{\alpha\beta}(\tau,\tau') = -\langle T_\tau\,\psi_\alpha(\tau)\psi_\beta^\dagger(\tau')\rangle \equiv -\mathrm{Tr}\left[T_\tau\,\underbrace{e^{-\beta(H-F)}}_{e^{-\int_0^\beta (H-?)\,d\tau''}}\psi_\alpha(\tau)\psi_\beta^\dagger(\tau')\right]$$

Consider: $H = \sum_\alpha \varepsilon_\alpha \psi_\alpha^\dagger\psi_\alpha$

$$\langle\psi_\alpha^\dagger\psi_\beta\rangle = \delta_{\alpha\beta}\,n(\varepsilon_\alpha)\;;\quad \varepsilon_\alpha = E_\alpha-\mu \qquad \text{—— (1)}$$

$n(\varepsilon_\alpha) \to n_F\,/\,n_B$

Evolution
$$\begin{cases}\psi_\alpha(\tau) = e^{-\varepsilon_\alpha\tau}\psi_\alpha\\ \psi_\alpha^\dagger(\tau) = e^{\varepsilon_\alpha\tau}\psi_\alpha^\dagger\end{cases}$$

$$G_{\alpha\beta}(\tau,\tau') = -\left[\theta(\tau-\tau')\langle\psi_\alpha\psi_\beta^\dagger\rangle \pm \theta(\tau'-\tau)\langle\psi_\beta^\dagger\psi_\alpha\rangle\right]e^{-\varepsilon_\alpha(\tau-\tau')}\delta_{\alpha\beta} \qquad \text{—— (2)}$$

$\downarrow$

$$G_{\alpha\beta}(\tau-\tau') \longrightarrow G_{\alpha\beta}(\tau) \equiv -\mathrm{Tr}\left[T_\tau e^{-\beta(H-F)}\psi_\alpha(\tau)\psi_\beta^\dagger(0)\right]$$

Property: $\boxed{G_{\alpha\beta}(\tau) = \pm G_{\alpha\beta}(\tau+\beta)}$ Periodicity / Anti-periodicity

Consider Bosonic case:

Period of $\tau = \frac{2\pi}{\beta}$ $\Longrightarrow$ Fourier Series $G_{\alpha\beta}(\tau) = T\sum_m G_{\alpha\beta}(i\Omega_m)e^{-i\Omega_m\tau}$

$$\boxed{\Omega_m = \frac{2\pi}{\beta}m\;;\; m\in\mathbb{Z}} \qquad G_{\alpha\beta}(i\Omega_m) = \int_0^\beta G_{\alpha\beta}(\tau)e^{i\Omega_m\tau}\,d\tau$$

$|||^{ly}$ $\boxed{\omega_n = \frac{2\pi}{\beta}\left(n+\frac{1}{2}\right)\;,\; n\in\mathbb{Z}}$ Matsubara Frequencies

$$\boxed{\begin{aligned}&\text{\&}\quad G_{\alpha\beta}(i\omega_n) = \delta_{\alpha\beta}\int_0^\beta d\tau\, e^{i\omega_n\tau}e^{-\varepsilon_\alpha\tau}n(\varepsilon_\alpha) = \delta_{\alpha\beta}\frac{1}{i\omega_n-\varepsilon_\alpha}\\ &|||^{ly}\quad G_{\alpha\beta}(i\Omega_m) = \delta_{\alpha\beta}\frac{1}{i\Omega_m-\varepsilon_\alpha}\end{aligned}}$$

Statistics absorbed in Ω_m/ω_n

$$\frac{\partial F}{\partial \mu} = -N \qquad \left.\begin{aligned} \hat{N}_\alpha &= T\sum_n \sum_\alpha G_{\alpha\alpha}(i\omega_n)e^{i\omega_n 0^+} \\ F &= -T\sum_n \sum_\alpha \ln\left[-G^{-1}_{\alpha\alpha}(i\omega_n)\right] e^{i\omega_n 0^+} \end{aligned}\right\}$$ Thermodynamics

$$\Downarrow$$

$$F = -T\sum_n \mathrm{Tr}\ln\left[-G^{-1}_{\alpha\beta}(i\omega_n)\right] e^{i\omega_n 0^+}$$

Spectral Decomposition of $G_{\alpha\beta}(i\omega_n)$

$$\Sigma \quad \left.\begin{aligned} \langle C_\alpha(t) C^\dagger_\beta(0)\rangle &= \int \frac{d\omega}{2\pi} G^>_{\alpha\beta}(\omega) e^{-i\omega t} \\ \& \quad \langle C^\dagger_\beta(0) C_\alpha(t)\rangle &= \int \frac{d\omega}{2\pi} G^<_{\alpha\beta}(\omega) e^{-i\omega t} \end{aligned}\right\} \Longrightarrow \quad G^>_{\alpha\beta}(\omega) = \sum_{a,b} P_b\, \rho^\alpha_{ba}\, \rho^{\dagger\beta}_{ab}\, \delta[E_a - E_b - \omega]$$

$$G^<_{\alpha\beta}(\omega) = \sum_{a,b} P_b\, \rho^{\dagger\beta}_{ba}\, \rho^\alpha_{ab}\, \delta[E_b - E_a - \omega]$$

$$G^R_{\alpha\beta}(t) = -i\langle\{C_\alpha(t), C^\dagger_\beta(0)\}\rangle\theta(t) = \int\frac{d\omega}{2\pi} G^R_{\alpha\beta}(\omega) e^{-i\omega t}$$

$\Updownarrow$ Real time analogue

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$$G_{\alpha\beta}(\tau) = -\langle T_\tau C_\alpha(\tau) C^\dagger_\beta(0)\rangle = T\sum_n G(i\omega_n) e^{-i\omega_n\tau}$$

can be written as

$$G_{\alpha\beta}(z) = \int d\omega \frac{1}{z-\omega} A_{\alpha\beta}(\omega)$$

$$\left.\begin{aligned} &\hookrightarrow z = \omega + i\delta \rightarrow G^R_{\alpha\beta}(\omega) \\ &z = i\omega_n \rightarrow G_{\alpha\beta}(i\omega_n) \end{aligned}\right]$$ dynamics related to Thermal averages.

Green's functions

$$A(\omega) = \frac{1}{2\pi}\left[G^>(\omega) + G^<(\omega)\right]$$

Finite T

Fermion

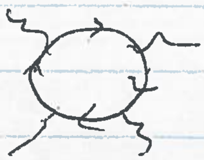
$$G^>(\omega) = \frac{2\pi}{1+e^{-\beta\omega}} A(\omega) \qquad \text{[Empty states]}$$

$$G^<(\omega) = \frac{2\pi}{1+e^{\beta\omega}} A(\omega) \qquad \text{[Filled States]}$$

Feynman Rules:

 $= G_0(k, i\omega_n)$

 $= -V(q)$

 $= [-(2S+1)]^F$

$T\sum_n \int \frac{d^dq}{(2\pi)^d}$ "internal variables summed over"

Next: → Evaluation of diagrams

→ Matsubara Sums Ex Hartree Fock / Polarization Bubble

→ Fluctuation Dissipation theorem / Experimental Quantities / KK relations

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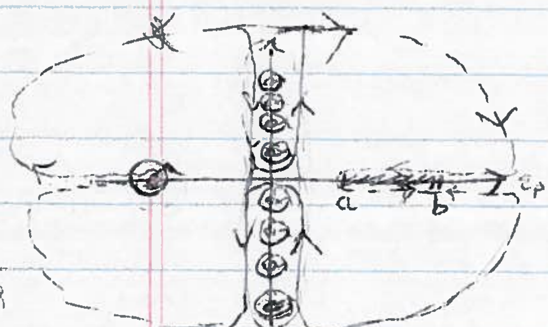
Matsubara Sums

$$T\sum_n F(i\omega_n) = -\oint_{C_1} \frac{dz}{2\pi i} F(z) f(z) \qquad \frac{-1}{1+e^z} \Big/ \frac{1}{1-e^z}$$

F / B



$$= \mp f(\epsilon_p) + \int_a^b d\epsilon \, [F(\epsilon^-) - F(\epsilon^+)] f(\epsilon)$$

$$\boxed{\text{Ex: } N = T\sum_n G(i\omega_n) e^{i\omega_n 0^+} = f(\epsilon_p)}$$

Further examples

(1) finite temp H-F:

$$T\sum_n \int \frac{d^d k}{(2\pi)^d} \equiv \int_K$$

$$\sum_\alpha \int_K G_{\alpha\alpha}(K) \sum_\beta \int_{K'} G_{\beta\beta}(K')\,(-1)^2\, V(0)$$

$$+ \sum_{\alpha,\beta} \int_K \int_{K'} G_{\alpha\beta}(K)\, G_{\beta\alpha}(K') \qquad (-1)\, V(K-K')$$

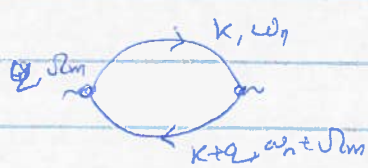
$$= \int_K \int_{K'} G(K)G(K')\left\{ -V(K-K')(2S+1) + (2S+1)^2 V(0) \right\}$$

$$\boxed{E_{HF} = \int_{\vec k}\int_{\vec k'} \left\{ (2S+1)^2 V(0) - V(\vec k-\vec k')(2S+1) \right\} f(\varepsilon_{\vec k}) f(\varepsilon_{\vec k'})}$$

(2) Impurity  $\Sigma(i\omega_n) = n_i u_0^2 \sum_{k'} \dfrac{1}{i\omega_n - \varepsilon_{k'} - \Sigma(i\omega_n)}$

$$= -i\frac{1}{2\tau}\,\mathrm{sgn}(\omega_n)$$

$$\frac{1}{2\tau} = n_i u_0^2 \nu_F$$

(3) 

$$\chi^{ab}(Q) = -\int_K \left[\sigma^a_{\alpha\beta} G_{\beta\gamma}(K) \sigma^b_{\gamma\delta} G_{\delta\alpha}(K+Q)\right]$$

$$= -2\delta^{ab} \int_K G(K)G(K+Q)$$

$$= -2\delta^{ab}\, \Pi(Q)$$

$$\Pi(Q) = T\sum_n \int_{\vec k} \frac{G(k) - G(k+q)}{i\Omega_m + \varepsilon_{\vec k} - \varepsilon_{\vec k+\vec q}} = \int_{\vec k} \frac{n(\varepsilon_k) - n(\varepsilon_{k+q})}{i\Omega_m + \varepsilon_{\vec k} - \varepsilon_{k+q}}$$

$$\Pi(\vec q, \Omega_m) \to \boxed{\Pi(\vec q, z)} \quad \text{Analytic continuation of } z$$

$$\to \Pi(\vec q, \Omega + i\delta)$$

$$\boxed{\Pi''(q,\Omega) = \int_{\vec k} \delta(\varepsilon_k - \varepsilon_{k+q} - \Omega)\left[n(\varepsilon_k) - n(\varepsilon_{k+q})\right]}$$ spectral form.

~~KK~~ relations

Fluctuation Dissipation Theorem: Chapter 9.

① $S(t-t') = \langle \hat{A}(t), A(t') \rangle = \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')} S(\omega)$

① $\chi(t-t') = i \langle [A(t), A(t')] \rangle \, \theta(t-t')$

Scratch

standard for $\langle A(t) \rangle = \int_{-\infty}^{\infty} dt' \, \chi(t-t') f(t') \quad ; \quad H_c = -f(t) A(t)$

$= \int dt' \; i \langle [A(t), A(t')] \rangle \, \theta(t-t') f(t')$

$= \int_{-\infty}^{t} dt' \; i \langle [A(t), A(t')] \rangle f(t')$

Causality ← $\boxed{\langle A(t) \rangle = i \int_{-\infty}^{t} \langle [A(t), H_c(t')] \rangle \, dt'}$ L. R. Theory

$A(t) = 1$ if $t \to -\infty$ when it was perturbed. $A(t)$ evolves from $-\infty$ upto t.

$i[H_c, A]$

$-i\langle [A(t), A(t')] \rangle f(t')$

$\Rightarrow \langle A(\omega) \rangle = \chi(\omega) f(\omega)$

Linear Response Theory.

$H_c(t') = A(t) f(t)$

Any response: $\langle A(t) \rangle = i \int_{-\infty}^{t} dt' \langle [H_c(t'), A(t)] \rangle$

Causality

$= -i \int_{-\infty}^{t} dt' \langle [A(t), A(t')] \rangle f(t')$

$= -i \int_{-\infty}^{\infty} dt' \langle [A, A'] \rangle \, \theta(t-t') f(t')$

$= \int_{-\infty} \chi(t-t') f(t')$

$\boxed{\langle A(\omega) \rangle = \chi(\omega) f(\omega)}$

$\chi(t-t') = -i \langle [A(t), A(t')] \rangle \, \theta(t-t')$

Finite Temperature:

$$\chi(t-t') = -i\langle [A(t), A(t')]\rangle\, \theta(t-t') \qquad \text{(Retarded)}$$

Let's add $\theta(t'-t)$

$$-i\langle [A(t), A(t')]\rangle\, \theta(t'-t) \qquad \text{(Advanced)}$$

allows.

$$\chi(\tau-\tau') = -\langle T_\tau A(\tau), A(\tau')\rangle$$

$$S(t-t') = \langle A(t), A(t')\rangle \qquad \text{Correlation, No Time order}$$

$$\boxed{S(\Omega) = 2\,[1+n_B(\Omega)]\,\chi''(\Omega)}$$

Fluctuation

Dissipation → Dissipative part of Response function

When $\omega \ll k_B T$, $\boxed{S(\omega) \simeq \frac{2T}{\omega}\chi''(\omega)}$

$$\langle A(t)\rangle = \int_{-\infty}^{\infty} \chi(t-t') f(t')\,dt' \qquad \langle A(\tau)\rangle = \int_0^{\beta} \chi(\tau-\tau') f(\tau')\,d\tau'$$

$$\chi(t-t') \equiv \chi_R(t-t') = i\langle [A(t), A(t')]\rangle\, \theta(t-t') \qquad \chi(\tau-\tau') = \langle T_\tau A(\tau), A(\tau')\rangle$$

$$\chi_A(t-t') = i\langle [A(t'), A(t)]\rangle\, \theta(t'-t)$$

$$= -i\langle [A(t), A(t')]\rangle\, \theta(t'-t)$$

$$S(t-t') = \langle A(t)\, A(t')\rangle = \sum_{\lambda} \langle \lambda | e^{-\beta(H-F)} A(t) A(t') | \lambda\rangle$$

$$= \sum_{\lambda\lambda'} \langle \lambda | A(t) | \lambda'\rangle \langle \lambda' | A(t') | \lambda\rangle\, e^{-\beta(E_\lambda - F)}$$

$$= \sum_{\lambda\lambda'} |\langle \lambda | A | \lambda'\rangle|^2 e^{i(E_\lambda - E_{\lambda'})(t-t')} e^{-\beta(E_\lambda - F)}$$

$$\boxed{S(\omega) = \sum_{\lambda\lambda'} e^{-\beta(E_\lambda - F)} |A_{\lambda\lambda'}|^2\, 2\pi\, \delta(E_\lambda - E_{\lambda'} - \omega)}$$

Spectrum of fluctuations

$$\chi(t-t') = i\langle [A(t), A(t')]\rangle\, \theta(t-t')$$

$$= i\sum_{\lambda\lambda'} e^{\beta F}\left(e^{-\beta E_\lambda} - e^{-\beta E_{\lambda'}}\right) |A_{\lambda\lambda'}|^2 e^{i(E_\lambda - E_{\lambda'})(t-t')}\, \theta(t-t').$$

$$\chi(\omega) = i\sum_{\lambda\lambda'} e^{-\beta(E_\lambda - F)}\left(1 - e^{-\beta\omega}\right) |A_{\lambda\lambda'}|^2 \underbrace{\int_{-\infty}^{\infty} dt\, e^{i(E_\lambda - E_{\lambda'} + \omega)t}\, \theta(t)}_{\frac{i}{\omega + i\delta + E_\lambda - E_{\lambda'}}}.$$

Proves F/D Theorem.

$$\boxed{\chi''(\omega) = \pi \sum_{\lambda\lambda'} e^{-\beta(E_\lambda - F)} \left(1 - e^{-\beta\omega}\right) |A_{\lambda\lambda'}|^2 \delta(\omega + E_\lambda - E_{\lambda'}).}$$

$\Downarrow$ Spectral Function

$$\chi_R(t) = \int \frac{d\omega}{2\pi} [2\chi''(\omega)]\, e^{-i\omega t}\, \theta(t)\, (i)$$

$$\chi_R(\omega) = \int \frac{d\omega'}{2\pi} \frac{1}{\omega' - \omega - i\delta} [2\chi''(\omega')]$$

$$\boxed{\chi(z) = \int \frac{d\omega'}{2\pi} \frac{1}{\omega' - z}\, 2\chi''(\omega')}$$

$z \to \omega + i\delta \quad \Rightarrow \chi_R(\omega)$

$z \to i\Omega_m \quad\quad \chi(i\Omega_m) \Rightarrow$ F.T. of $\chi(\tau - \tau')$

$$\boxed{\chi''(\Omega) = \frac{\chi(\omega + i\delta) - \chi(\omega - i\delta)}{2i}}$$

Branch cut.

Apply the same to fermions $[A(t), A(t')] \Downarrow [c(t), c^{+}(t')]$

$$\boxed{G_{\alpha\beta}(z) = \int \frac{d\omega}{2\pi} \frac{1}{z-\omega} A_{\alpha\beta}(\omega)}$$

$$A_{\alpha\beta}(\omega) \equiv G^{\prime\prime}_{\alpha\beta}(\omega) = \frac{G(\omega+i\delta) - G(\omega-i\delta)}{2i}$$

$$A(\omega) = [G^{>}(\omega) + G^{<}(\omega)].$$

$$G^{>}(\omega) = \frac{e^{\beta\omega}}{1+e^{\beta\omega}} G^{\prime\prime}_{\alpha\beta}(\omega) \quad \text{[empty state]}$$

$$G^{<}(\omega) = \frac{1}{1+e^{\beta\omega}} G^{\prime\prime}_{\alpha\beta}(\omega) \quad \text{[filled state]}.$$

Experimental Quantities

STM: $\frac{dI}{dV} \propto A(x,\omega)$ (local)

ARPES: $I(k,\omega) \propto f(\omega) A(k,\omega)$.

Charge: $\sigma(\omega) = \frac{1}{-i\omega} \langle j(\omega) j(-\omega) \rangle$.

$$\rho = \frac{1}{\sigma(0)}$$

Spin. $\chi_{DC} = \int \frac{d\omega}{\pi} \frac{1}{\omega} \chi''(\omega)$

INS $S(q,\omega) = e^{\beta\omega} n_B(\omega) \chi''(q,\omega)$.

Key ingredient from ~~spectral Analysis~~ finite T:
existence of spectral function.

$G(z), \chi(z)$

can be got from spectral functions.
$G''(z)$; $\chi''(z)$

$z = \Omega + i\delta$ → Retarded functions — Needed in real response

$z = i\Omega_n$ → Analogous to $T=0$ Calculation; Needed for diagrams

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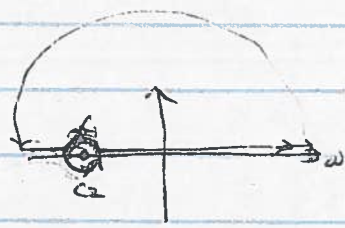
What are KK relations?

K.R. relations:

Spectral function

$$\chi'(\omega) = P\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi''(\omega')}{\omega'-\omega} \longrightarrow \chi(z) = \int \frac{d\omega}{\pi} \frac{\chi''(\omega')}{\omega'-z}$$

$$\chi''(\omega) = -P\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi'(\omega')}{\omega'-\omega}$$



$$\chi(\omega) = \oint \frac{\chi(\omega')}{\omega'-\omega} \frac{d\omega'}{2\pi i} = -2\int_{c_1}$$

$$\int_{c_1} = -P\int_{-\infty}^{\infty}$$

$$\therefore \boxed{\chi(\omega) = P\int_{-\infty}^{\infty} \frac{d\omega'}{\pi i} \frac{\chi(\omega')}{\omega'-\omega}}$$

What functions do this?

No poles on one ½ plane

after fluctuation dissipation theorem } "Retarded functions" "Causal"