Chap. 3: Fcts de Green

Shrödinger à 1 corps.

$\hbar = 1$

1. Déf. de G

2. Information contenue dans G

- Repr. opétateur
- Relation à $\rho(\omega)$
- Repr. spetrale, règles de somme, dév $\omega \to \infty$
- Relation au transport
- Green pour e.d.

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$$\Psi(r,t) = \langle r | e^{-iHt} | \Psi_H \rangle$$

$$|\Psi_0(t')\rangle = e^{-iHt'} |\Psi_H\rangle$$

$$\Psi(r,t) = \langle r | e^{-iH(t-t')} | \Psi_0(t') \rangle$$

$$\int |r'\rangle\langle r'|$$

$$\Psi(r,t) = \int d^3r' \, \langle r | e^{-iH(t-t')} | r' \rangle \, \Psi_0(r',t')$$

$$\theta(t-t')\,\Psi(r,t) = i \int d^3r' \, G^R(r,t\,;r',t')\,\Psi_0(r',t')$$

$$\boxed{G^R(r,t\,;r',t') \equiv -i \langle r | e^{-iH(t-t')} | r' \rangle \, \theta(t-t')}$$

Fct. de Green

Propagateur

- Information dans G^R

$$G^R(r,r';\omega) = -i\int_0^\infty d(\underbrace{t-t'})\, e^{i(\omega+i\eta)(\underbrace{t-t'})}$$

$$\langle r|\, e^{-iH\,(\underbrace{t-t'})}\, |r'\rangle$$

$$H|n\rangle = E_n|n\rangle \qquad \uparrow \sum_n |n\rangle\langle n|$$

$$= -i\int_0^\infty dt\, e^{+i(\omega+i\eta)t} \sum_n \langle r|\, e^{-iE_n t}|n\rangle\langle n|r'\rangle$$

$$= -i\sum_n \left.\frac{e^{+i(\omega+i\eta)t}}{+i(\omega+i\eta)-iE_n}\right|_0^\infty \langle r|n\rangle\langle n|r'\rangle$$

$$\to \mathrm{Im}\, G^R(r,r;\omega) = -\pi\sum_n \langle r|n\rangle\langle n|r\rangle\, \delta(\omega-E_n)$$

$$\boxed{= \sum_n \frac{\langle r|n\rangle\langle n|r'\rangle}{\omega+i\eta-E_n} \qquad G^R(r,r';\omega) = \sum_n \frac{\psi_n(r)\,\psi_n^*(r')}{\omega+i\eta-E_n}}$$

- Pôles aux énergies propres
- Résidus dépendent des $\psi_n(r)$

Repr. Lehman

Repr. spectrale.

$$\sum_{n'}\sum_n \langle r|n\rangle\langle n|\frac{1}{\omega+i\eta-H}|n'\rangle\langle n'|r'\rangle$$

$$= \langle r|\frac{1}{\omega+i\eta-H}|r'\rangle$$

Repr. en opérateurs.

$$\boxed{\hat{G}^R(\omega) = \frac{1}{\omega+i\eta-H}} \quad \text{Résolvant}$$

$$G^R(r,r';\omega) = \langle r|\, \hat{G}^R(\omega)\, |r'\rangle$$

$$\hat{G}^R(t) = -i\, e^{-iHt}\,\theta(t)$$

$$\boxed{\hat{G}^A(t) = i\, e^{-iHt}\,\theta(-t)}$$

$$\hat{G}^A(\omega) = \frac{1}{\omega - i\eta - H}$$

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Relation à la densité d'états

$$\rho(E) \equiv \sum_n \delta(E - E_n)$$

$$= \sum_n \int d^3r \, \underline{\langle n | r \rangle \langle r | n \rangle \delta(E-E_n)}$$

$$= -\frac{1}{\pi} \int dr \, \mathrm{Im}\, G^R(r, r; E)$$

$$\boxed{\rho(E) = -\frac{1}{\pi} \mathrm{Tr} \left[\mathrm{Im}\, \hat{G}^R(E) \right]}$$

$$\rho(r, E) = -\frac{1}{\pi} \mathrm{Im}\, G^R(r, r; E)$$

$\uparrow$ DOS locale.

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Repr. spectrale.

$$G^R(r,r';\omega) = \int \frac{d\omega'}{2\pi} \frac{\boxed{A(r,r';\omega')}}{\omega + i\eta - \omega'}$$

$$= \int \frac{d\omega'}{2\pi} \frac{\boxed{-2\,\mathrm{Im}\, G^R(r,r';\omega')}}{\omega + i\eta - \omega'}$$

Analogue:

$$\chi^R(\omega) = \int \frac{d\omega'}{\pi} \frac{\chi''(\omega')}{\omega' - \omega - i\eta}$$

Preuve:

$$G^R(r,r';\omega) = \sum_n \frac{\Psi_n(r)\Psi_n^*(r')}{\omega + i\eta - E_n}$$

$$= \int \frac{d\omega'}{2\pi} \frac{\boxed{\sum_n \delta(\omega' - E_n)\Psi_n(r)\Psi_n^*(r')\, 2\pi}}{\omega + i\eta - \omega'}$$

$$G^R(\vec{k},\omega) = \int \frac{d\omega'}{2\pi} \frac{A(k,\omega')}{\omega + i\eta - \omega'}$$

Règles de somme

$A(r,r';\omega)$

Poids spectral

$$\int \frac{d\omega'}{2\pi} \left(-2\,\mathrm{Im}\, G^R(r,r';\omega)\right)$$

$$= \int \frac{d\omega'}{2\pi} \left(\sum_n \Psi_n(r) \Psi_n^*(r')\, 2\pi\, \delta(\omega' - E_n) \right)$$

$$= \sum_n \Psi_n(r) \Psi_n^*(r') = \langle r | r' \rangle = \delta(r - r')$$

$$\int d^3r \int \frac{d\omega'}{2\pi}\, \omega' \left(-2\,\mathrm{Im}\, G^R(r,r,\omega')\right)$$

$$\int d^3r \sum_n E_n \Psi_n(r) \Psi_n^*(r)$$

Avec $r = r'$

$$\underbrace{\int d^3r \, \langle r | H | r \rangle}_{} = \sum_n \int d^3r \, \langle r | n \rangle \langle n | H | n \rangle \langle n | r \rangle$$

$$\int \frac{d\omega}{2\pi}\, \omega^n \, \mathrm{Tr}\left[-2\,\mathrm{Im}\, \hat{G}^R\right]$$

$$= \int \frac{d\omega}{2\pi}\, \omega^n \, \mathrm{Tr}\left[-2\,\mathrm{Im}\, \frac{1}{\omega + i\eta - H}\right]$$

$$= \int \frac{d\omega}{\cancel{2\pi}}\, \omega^n \, \mathrm{Tr}\left[-\cancel{2}(-\cancel{\pi})\, \delta(\omega - H)\right]$$

$$= \mathrm{Tr}\, H^n = \int d^3r \, \langle r | H^n | r \rangle$$

$$= \int \frac{d^3k}{(2\pi)^3} \langle k | H^n | k \rangle \longleftarrow$$

Dév. $\omega \to \infty$

$$G^R(k,k;\omega) = \int \frac{d\omega'}{2\pi} \frac{-2\,\mathrm{Im}\,G^R(k,\omega')}{\omega + i\eta - \omega'}$$

$\omega \to \infty$

$$= \sum_{n=0}^{\infty} \frac{1}{\omega^{n+1}} \int d\omega' (\omega')^n \left(-2\,\mathrm{Im}\,G^R(k,\omega')\right)$$

$$\int \frac{d^3k}{(2\pi)^3} (\quad) = \sum_{n=0}^{\infty} \frac{1}{\omega^{n+1}} \int \frac{d^3k}{(2\pi)^3} \langle k | H^n | k \rangle$$

$$= \sum_{n=0}^{\infty} \frac{1}{\omega^{n+1}} \mathrm{Tr}\,(H^n)$$

$$\hat{G}^R(\omega) = \frac{1}{\omega + i\eta - H}$$

Relation au transport et aux fluctuations

$$S_{\rho\rho}(k,\omega) = \frac{1}{V}\int dt\, e^{i\omega t} \langle \rho_k(t)\rho_{-k}(0)\rangle$$

$$\to \quad = \frac{1}{V}\int dt\, e^{i\omega t} \langle e^{iHt} \rho_k e^{-iHt} \rho_{-k}\rangle$$

$$\hat{G}^R(t) = -i e^{-iHt}\theta(t) \; , \quad \hat{G}^A(t) = i e^{-iHt}\theta(-t)$$

$$= -\frac{1}{V}\int dt\, e^{i\omega t} \langle \left(\hat{G}^R(-t) - \hat{G}^A(-t)\right)\rho_k \left(\hat{G}^R(t) - \hat{G}^A(t)\right)\rho_{-k}\rangle$$

$$G^R(t)\,G^R(-t) = 0$$

$$\theta(t)\theta(-t) = 0$$

$$= \frac{1}{V}\int dt\, e^{i\omega t} \langle \hat{G}^R(-t)\rho_k \hat{G}^A(t)\rho_{-k} + \hat{G}^A(-t)\rho_k G^R(t)\rho_{-k}\rangle$$

$$S(k,\omega) = \frac{1}{V}\int \frac{d\omega'}{2\pi} \langle \hat{G}^R(\omega')\rho_k \hat{G}^A(\omega'+\omega)\rho_{-k} + A \leftrightarrow R\rangle$$

Fcts de Green et E.Diff.

$$\tilde{G}^R = G_0^R + G_0^R V G_0^R \ldots\ldots$$

$\hat{H}$ $\quad \hat{G}^R = \dfrac{1}{\omega + i\eta - \hat{H}} =$

$\hat{H} = \hat{H}_0 + \hat{V} \qquad \dfrac{1}{\omega + i\eta - H_0}$

$$\langle k | \hat{G}^R | k \rangle = \frac{1}{\omega + i\eta - \epsilon_k - \Sigma(k,\omega)}$$

$$\Sigma(k,\omega) \longrightarrow \frac{1}{\tau}$$

$$\chi_{jj} \rightarrow \sigma \rightarrow \frac{ne^2\tau}{m}$$

$$\boxed{\Psi(r,t)\,\theta(t-t') = i\int d^3r'\, G^R(r,t;r't')\,\Psi_0(r',t')}$$

$$i\frac{\partial}{\partial t}\left[\Psi\theta\right] = i\delta(t-t')\,\Psi(r,t)$$

$$+ H\,\Psi(r,t)\,\theta(t-t')$$

$\Psi(r,t')=\Psi_0(r,t')$

$\int dr' |r'\rangle\langle r'|$

$$\boxed{i\frac{\partial}{\partial t}\Psi = H(r)\Psi} \qquad i\frac{\partial}{\partial t}\langle r|\Psi\rangle = \langle r|H|\Psi\rangle$$

$$i\frac{\partial}{\partial t}\left[i\int d^3r'\, G^R(r,t;r',t')\,\Psi_0(\cancel{r'},t')\right]$$

$$= i\delta(t-t')\int d^3r'\,\delta(r-r')\,\Psi_0(\cancel{r'},t')$$

$$H(r)\left[i\int d^3r'\, G^R(r,t;r',t')\,\Psi_0(\cancel{r'},t')\right]$$

$$\boxed{\left[i\frac{\partial}{\partial t} - H\right] G^R(r,t;r',t') = \delta(t-t')\,\delta^3(r-r')}$$

Opérateur

$$\hat{G}^R(t) = -i\, e^{-iHt}\,\Theta(t)$$

$$\boxed{\left[i\frac{\partial}{\partial t} - H\right]\hat{G}^R = \delta(t)}$$

$$\boxed{\hat{G}^{R(A)} = \frac{1}{i\frac{\partial}{\partial t} - H}\,\delta(t)}$$

$$\hat{G}^R(\omega) = \frac{1}{\omega + i\eta - H} \qquad \hat{G}^A = \frac{1}{\omega - i\eta - H}$$

Sol. Générale:

$$\boxed{-i\,\Theta(t)\,e^{-iHt} + C\,e^{-iHt}}$$

$$G^A \Rightarrow -i + C = 0 \Rightarrow C = i$$

$$-i\,\Theta(t)\,e^{-iHt} + i\,e^{-iHt} = i\,e^{-iHt}\,\Theta(-t)$$