Luttinger-Ward Functional in the Closed Time Path Formalism

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§. Nonlocal S Matrix

$$S \equiv \underbrace{T}_{}\overset{\exp}{[}-\frac{i}{\hbar}\sum_{\sigma}\int_p d1\int_p d1'\, \psi^{+}_{H\sigma}(1)\phi(1,1')\psi_{H\sigma}(1')\ ] \qquad (1)$$

§. Response Theorems

$$\text{(A)}\quad \frac{\delta S}{\delta\phi(2,2')} = -\frac{i}{\hbar}\sum_{\sigma} T[\psi^{+}_{H\sigma}(2)\psi_{H\sigma}(2')S] \qquad (2)$$

$$\text{(B)}\quad \frac{\delta\langle T[A(t)B(t')\cdots]\rangle}{\delta\phi(2,2')} = -\frac{i}{\hbar}\sum_{\sigma}\langle T\{\delta[\psi^{+}_{\sigma}(2)\psi_{\sigma}(2')]A(t)B(t')\cdots\}\rangle \qquad (3)$$

where

$$\delta[\psi^{+}_{\sigma}(2)\psi_{\sigma}(2')] = \psi^{+}_{\sigma}(2)\psi_{\sigma}(2') - \langle\psi^{+}_{\sigma}(2)\psi_{\sigma}(2')\rangle \qquad (4)$$

$$\langle O(t)\rangle = \mathrm{tr}\{T[O_H(t)S]\rho\}/\mathrm{tr}[S\rho] \qquad (5)$$

∵ (A) $$\frac{\delta}{\delta\phi(2,2')}\sum_{n=0}^{\infty}\left(-\frac{i}{\hbar}\right)^n\sum_{\sigma_1\cdots\sigma_n}\int d1\int d1'\cdots\int dn\int dn'\,\phi(11')\cdots\phi(nn')\,T[\psi^{+}_{\sigma_1}(1)\psi_{\sigma_1}(1')\cdots\psi^{+}_{\sigma_n}(n)\psi_{\sigma_n}(n')]$$

$$= \sum_{n=1}^{\infty}\frac{1}{(n-1)!}\left(-\frac{i}{\hbar}\right)^n\sum_{\sigma_1\cdots\sigma_n}\int d2\int d2'\cdots\int dn\int dn'\,\phi(22')\cdots\phi(nn')$$
$$\times T[\psi^{+}_{\sigma_1}(2)\psi_{\sigma_1}(2')\psi^{+}_{\sigma_2}(2)\psi_{\sigma_2}(2)\cdots\psi^{+}_{\sigma_n}(n)\psi_{\sigma_n}(n')]$$

$$= -\frac{i}{\hbar}\sum_{\sigma}T[\psi^{+}_{\sigma}(2)\psi_{\sigma}(2)S] \qquad //$$

§. Generating Functional

$$Z \equiv \mathrm{tr}[S\rho] \tag{6}$$

$$W \equiv -\frac{\hbar}{2} \ln Z \tag{7}$$

Then,

$$\frac{\delta W}{\delta \Phi(1',1)} = \mathcal{G}(1,1') \tag{8}$$

where the single-particle Green's function is defined as

$$\mathcal{G}(1,1') = -\frac{i}{2}\sum_{\sigma}\langle T[\psi_\sigma(1)\psi_\sigma^+(1')]\rangle \tag{9}$$

$$\because \frac{\delta W}{\delta \Phi(1',1)} = -\frac{\hbar}{2}\frac{\mathrm{tr}\{[\delta S/\delta\Phi(1',1)]\rho\}}{\mathrm{tr}[S\rho]}$$

additional minus sign

$$= +\frac{\hbar}{2}\left(+\frac{i}{\hbar}\right)\sum_{\sigma}\frac{\mathrm{tr}\{T[\psi_\sigma^+(1')\psi_\sigma(1)S]\rho\}}{\mathrm{tr}[S\rho]}$$

$$= -\frac{i}{2}\sum_{\sigma}\langle T[\psi_\sigma(1)\psi_\sigma^+(1')]\rangle \quad //$$

§. Vertex Functional

By performing the Legendre transform, we define the vertex functional Γ as,

$$\Gamma[\mathcal{G}(1,1')] \equiv W[\Phi(1,1')] - \int_p d1\int_p d1' \mathcal{G}(1,1')\Phi(1',1) \tag{10}$$

Then,

$$\frac{\delta \Gamma}{\delta \mathcal{G}(1,1')} = -\Phi(1',1) \tag{11}$$

($\because$ $\delta\Gamma = \underbrace{\delta W}_{\int_p d1 \int_p d1' \cancel{g(1,1')\delta\Phi(1',1)}} - \int_p d1 \int_p d1' \,[\, \cancel{g(1,1')\delta\Phi(1',1)} + \delta g(1,1')\Phi(1',1) \,]$ //)

We define the ν-body vertex functions $\Gamma^{(\nu)}$ as the functional derivatives of Γ with respect to Green's functions,

$$\boxed{\Gamma^{(\nu)}(1,1';\ldots;\nu,\nu') \equiv \frac{\delta^{\nu}}{\delta g(\nu,\nu')\cdots\delta g(1,1')}\,\Gamma \qquad (12)}$$

§. Equation of Motion for the Green's Function

$$i\hbar\frac{\partial}{\partial t_1} g(1,1') = -\frac{i}{2}\sum_\sigma i\hbar\frac{\partial}{\partial t_1}\left\{\Theta_p(\underline{\underline{t_1}}-t_1')\langle\psi_\sigma(1)\psi_\sigma^{+}(1')\rangle - \Theta_p(t_1'-\underline{\underline{t_1}})\langle\psi_\sigma^{+}(1')\psi_\sigma(1)\rangle\right\}$$

$$= -\frac{i}{2}\sum_\sigma i\hbar\,\delta_p(t_1-t_1')\,\langle\underbrace{\{\psi_\sigma(r_1 t_1),\psi_\sigma^{+}(r_1',t_1)\}}_{\delta(r_1-r_1')}\rangle$$

$$-\frac{i}{2}\sum_\sigma \Theta_p(t_1-t_1')\, i\hbar\frac{\partial}{\partial t_1}\langle\cdots S_\pm(*,t_1)\psi_\sigma(\underline{\underline{1}})S_\pm(t_1,*)\cdots\rangle$$

$$+\frac{i}{2}\sum_\sigma \Theta_p(t_1'-t_1)\, i\hbar\frac{\partial}{\partial t_1}\langle\cdots S_\pm(*,t_1)\psi_\sigma(\underline{\underline{1}})S_\pm(t_1,*)\cdots\rangle \qquad (13)$$

※Note that the delta function here is defined as

$$\boxed{\delta_p(t-t') = \frac{d}{dt}\Theta_p(t-t') = \begin{cases}\delta(t-t') & \text{for } (t,t')\in(+,+) \\ -\delta(t-t') & (-,-) \\ 0 & \text{otherwise}\end{cases} \qquad (14)}$$

($\because$ On the minus path,

$$\frac{d}{dt}\underbrace{\Theta_p(t-t')}_{\Theta(t'-t)} = -\delta(t-t') \quad //$$
)

Noting that all t_1 dependence should be added *linearly*,

$$i\hbar\frac{\partial}{\partial t_\nu}\langle T\psi_\sigma(\nu)\underline{\underline{S}}\rangle$$

$$= i\hbar\frac{\partial}{\partial t_\nu}\sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n\sum_{\sigma_1\cdots\sigma_n}\int_p d1\int_p d1'\cdots\int_p dn\int_p dn'\,\phi(1,1')\cdots\phi(n,n')$$

$$\times\underbrace{T[\psi^+_{\sigma_1}(1)\psi_{\sigma_1}(1')\cdots\overset{+}{\psi^+_{\sigma_n}(n)}\overset{-}{\psi_{\sigma_n}(n')}\psi_\sigma(\nu)]}$$

$$n\times\left\{\begin{array}{l}\left[\cdots\left(\int_p^{t_\nu}dn\,\psi_\sigma(\nu)\psi^+_{\sigma_n}(n)-\int_{t_\nu}^{p}dn\,\psi^+_{\sigma_n}(n)\psi_\sigma(\nu)\right)\cdots\right]\\+\left[\cdots\left(-\int_p^{t_\nu}dn'\psi_\sigma(\nu)\psi_{\sigma_n}(n')+\int_{t_\nu}^{p}dn'\psi_{\sigma_n}(n)\psi_\sigma(\nu)\right)\cdots\right]\end{array}\right\}$$

$$=\sum_{n=1}^{\infty}\frac{1}{(n-1)!}\left(-\frac{i}{\hbar}\right)^{n-1}\sum_{\sigma_1\cdots\sigma_n}\int_p d1\int_p d1'\cdots\int_p d(n-1)\int_p d(n'-1)\,\phi(1,1')\cdots\phi(n-1,n'-1)$$

$$\underbrace{\times\left\{\begin{array}{l}\left[\cdots\int dr_n\int_p dn'\,\phi(r_n,t_\nu;n')\{\underbrace{\psi_\sigma(\nu),\psi^+_{\sigma_n}(r_n,t_\nu)}_{\delta_{\sigma\sigma_n}\delta(r_n-r_\nu)}\}\psi_{\sigma_n}(n')\cdots\right]\\-\left[\cdots\int_p dn\int dr_n'\,\phi(n;r_n',t_\nu)\,\psi^+_{\sigma_n}(n)\cancel{\{\psi_\sigma(\nu),\psi_{\sigma_n}(r_n',t_\nu)\}}\cdots\right]\end{array}\right\}}_{\int_p dn'\,\phi(\nu,n')\,\psi_\sigma(n')}$$

$$=\int_p dn'\,\phi(\nu,n')\,\langle T[\psi_\sigma(n')S]\rangle \tag{15}$$

Using Eq. (15), Eq. (13) can be rewritten as

$$i\hbar\frac{\partial}{\partial t_1}G(1,1')=\hbar\,\delta_p(1,1')-\frac{i}{2}\sum_\sigma\langle T\{[\psi_\sigma(1),H]S\}\rangle$$

$$+\int_p d2\,\phi(1,2)\,G(2,1') \tag{16}$$

(Commutators)

① $$[\psi_\sigma(r), T] = \sum_\lambda \int d^3x\, \underbrace{[\psi_\sigma(r), \overset{+}{\psi^\dagger_\lambda(x)} (-\frac{\hbar^2}{2m}\nabla_x^2)\psi_\lambda(x)]}_{\delta_{\sigma\lambda}\delta(r-x)(-\frac{\hbar^2}{2m}\nabla_x^2)\psi_\lambda(x)}$$

$$= -\frac{\hbar^2}{2m}\nabla^2\psi_\sigma(r) \qquad (17)$$

② $$[\psi_\sigma(r), U] = \frac{1}{2}\sum_{\lambda\lambda'}\int d^3x\int d^3x'\, v(x-x')\, \underbrace{[\psi_\sigma(r), \psi^\dagger_\lambda(x)\psi^\dagger_{\lambda'}(x')\psi_{\lambda'}(x')\psi_\lambda(x)]}$$

$$\delta_{\sigma\lambda}\delta(r-x)\psi^\dagger_{\lambda'}(x')\psi_{\lambda'}(x')\psi_\sigma(r)$$

$$-\psi^\dagger_\lambda(x)\delta_{\sigma\lambda}\delta(r-x)\psi_\sigma(r)\psi_\lambda(x)$$

$$= \cancel{\frac{1}{2}}\sum_\lambda\int d^3x\, v(r-x)\times\cancel{2}\, \psi^\dagger_\lambda(x)\psi_\lambda(x)\,\psi_\sigma(r)$$

$$= \int d^3x\, v(r-x)\rho(x)\psi_\sigma(r) \qquad (18)$$

Using Eqs. (17) and (18), Eq. (16) becomes

$$i\hbar\frac{\partial}{\partial t_1}G(1,1') = \hbar\delta_p(1,1') - \frac{\hbar^2}{2m}\nabla_1^2 G(1,1') - \frac{i}{2}\sum_\sigma\int d^3r_2\, v(r_1-r_2)\langle T[\underbrace{\rho(r_2,t_1)}_{\langle\rho(r_2,t_1)\rangle+\delta\rho(r_2,t_1)}\psi_\sigma(1)\psi^\dagger_\sigma(1')]\rangle$$

$$+\ \phi(1,\bar{2})G(\bar{2},1')$$

$$\left[i\frac{\partial}{\partial t_1} + \frac{\hbar}{2m}\nabla_1^2 - \frac{1}{\hbar}v(1,\bar{2})\langle\rho(\bar{2})\rangle\right]G(1,1') - \phi(1,\bar{2})G(\bar{2},1')$$

$$\underbrace{+\frac{i}{2\hbar}\sum_\sigma v(1^+,\bar{2})\langle T[\delta\rho(2)\psi_\sigma(1)\psi^\dagger_\sigma(1')]\rangle}\ = \delta_p(1,1')$$

$$-\frac{i}{2\hbar}\sum_\sigma v(1^+,\bar{2})\langle T[\delta\rho(2)\psi^\dagger_\sigma(1')\psi_\sigma(1)]\rangle$$

$$= \frac{1}{2}v(1^+,\bar{2})\underbrace{\frac{\delta}{\delta\phi(\bar{2}^+,\bar{2})}\sum_\sigma\langle T[\psi^\dagger_\sigma(1')\psi_\sigma(1)]\rangle}$$

$$\equiv \chi^{(2)}(1',1;2^+,2)$$

$$\left[i\frac{\partial}{\partial t_1}+\frac{\hbar}{2m}\nabla_1^2-\frac{1}{\hbar}v(1,\bar{2})\langle\rho(\bar{2})\rangle\right]\mathcal{G}(1,1')$$

$$-\frac{1}{\hbar}\Phi(1,\bar{2})\mathcal{G}(\bar{2},1')+\frac{1}{2}v(1^+,\bar{2})\chi^{(2)}(1',1;\bar{2}^+,\bar{2})=\delta_p(1,1') \tag{19}$$

Here,

$$v(1,2)=v(|r_1-r_2|)\,\delta_p(t_1-t_2) \tag{20}$$

$$1^+=(r_1,t_1+0_p) \tag{21}$$

and t_1+0_p is infinitesimaly later than t_1 on the path.

§. Response Functions

In Eq. (19), ν-body response functions are defined as

$$\chi^{(\nu)}(1,1';\ldots;\nu,\nu')=\frac{\delta^{\nu-1}}{\delta\Phi(\nu,\nu')\cdots\delta\Phi(2,2')}\sum_\sigma\langle T[\psi_\sigma^\dagger(1)\psi_\sigma(1')]\rangle \tag{22}$$

§. Self-Energy

Equation (19) can be rewritten as

$$\left[i\frac{\partial}{\partial t_1}+\frac{\hbar}{2m}\nabla_1^2-\frac{1}{\hbar}v(1,\bar{2})\langle\rho(\bar{2})\rangle\right]\mathcal{G}(1,1')$$

$$-\frac{1}{\hbar}\Phi(1,\bar{2})\mathcal{G}(\bar{2},1')-\Sigma(1,\bar{2})\mathcal{G}(\bar{2},1')=\delta_p(1,1') \tag{23}$$

where the self-energy is defined as

$$\Sigma(1,1')=-\frac{1}{2}v(1^+,\bar{2})\chi^{(2)}(\bar{3},1;\bar{2}^+,\bar{2})\mathcal{G}^{-1}(\bar{3},1') \tag{24}$$

§. Dyson's Equation

$$\left[i\frac{\partial}{\partial t_1}+\frac{\hbar}{2m}\nabla_1^2-\frac{1}{\hbar}v(1,\bar{2})\langle\rho(\bar{2})\rangle\right]\mathcal{G}(1,1')$$

$$=\delta_p(1,\bar{3})\left[\left(i\frac{\partial}{\partial t_3}+\frac{\hbar}{2m}\nabla_3^2\right)-\frac{1}{\hbar}v(\bar{3},\bar{2})\langle\rho(\bar{2})\rangle\right]\mathcal{G}(\bar{3},1')$$

$$=\underbrace{-i\frac{\partial}{\partial t_3}\delta_p(1,\bar{3})}_{=i\frac{\partial}{\partial t_1}\delta_p(1,\bar{3})}+\underbrace{\frac{\hbar}{2m}\nabla_3^2\delta_p(1,\bar{3})}_{=\frac{\hbar}{2m}\nabla_1^2\delta_p(1,\bar{3})}-\frac{1}{\hbar}v(1,\bar{2})\langle\rho(\bar{2})\rangle\delta_p(1,\bar{3})$$

$$=\left[\underbrace{\left(i\frac{\partial}{\partial t_1}+\frac{\hbar}{2m}\nabla_1^2\right)\delta_p(1,\bar{2})}_{\equiv\,\mathcal{G}_0^{-1}(1,\bar{2})}-\frac{1}{\hbar}v(1,\bar{3})\underbrace{\langle\rho(\bar{3})\rangle}_{-2i\mathcal{G}(\bar{3},\bar{3}^+)}\delta_p(1,\bar{2})\right]\mathcal{G}(\bar{2},1')$$

$$\mathcal{G}^{-1}(1,1')=\mathcal{G}_0^{-1}(1,1')-\frac{1}{\hbar}v(1,\bar{2})\langle\rho(\bar{2})\rangle\delta_p(1,1')-\frac{1}{\hbar}\phi(1,1')-\Sigma(1,1') \tag{25a}$$

$$=\mathcal{G}_0^{-1}(1,1')+\frac{2i}{\hbar}v(1,\bar{2})\mathcal{G}(\bar{2},\bar{2}^+)\delta_p(1,1')-\frac{1}{\hbar}\phi(1,1')-\Sigma(1,1') \tag{25b}$$

where

$$\mathcal{G}_0^{-1}(1,1')=\left(i\frac{\partial}{\partial t_1}+\frac{\hbar}{2m}\nabla_1^2\right)\delta_p(1,1') \tag{26}$$

$$\Sigma(1,1')=-\frac{1}{2}v(1^+,\bar{2})\chi^{(2)}(\bar{3},1;\bar{2}^+,\bar{2})\mathcal{G}^{-1}(\bar{3},1') \tag{24}$$

Comparing Eqs. (11) and (25b),

$$\frac{\delta\Gamma}{\delta G(1,1')} = \hbar G^{-1}(1',1) - \hbar G_0^{-1}(1',1) - 2i\, v(1^+,\bar{2}) G(\bar{2},\bar{2}^+) \delta_p(1',1) + \underline{\Sigma(1',1)} \tag{27}$$

Here, we introduce

$$\Gamma_0[G] = \hbar \int_p d1 \int_p d1' \ln G_0^{-1}(1',1) G(1,1') - \hbar \int_p d1 \int_p d1' G_0^{-1}(1',1) G(1,1')$$
$$- i\, v(\bar{1},\bar{2}) G(\bar{1},\bar{1}^+) G(\bar{2},\bar{2}^+)$$

then

$$\frac{\delta\Gamma_0}{\delta G(1,1')} = \hbar G(1',\bar{2}) \underbrace{G_0(\bar{2},\bar{2}') G_0^{-1}(\bar{2}',1)}_{\delta(\bar{2},1)} - \hbar G_0^{-1}(1',1) - i\, v(1,\bar{2}) G(\bar{2},\bar{2}^+) \delta_p(1^+,1')$$

Thus, Γ is decomposed into

$$\Gamma[G] = \Gamma_0[G] + \Gamma_H[G] + \Xi[G] \tag{28}$$

$$\Gamma_0[G] = \hbar \int_p d1 \int_p d1' \left[\ln G_0^{-1}(1,1') G(1',1) - G_0^{-1}(1,1') G(1',1) + 1 \right] \tag{29}$$

$$\Gamma_H[G] = - i\, v(\bar{1},\bar{2}) G(\bar{1},\bar{1}^+) G(\bar{2},\bar{2}^+) \tag{30}$$

and $\Xi[G]$ is the generator of the correlation potentials

$$\Xi^{(\nu)}(1,1';\ldots;\nu,\nu') = \frac{\delta^\nu}{\delta G(\nu,\nu')\cdots\delta G(1,1')}\, \Xi \tag{31}$$

In particular, $\Xi^{(1)}(1,1') = \Sigma(1,1')$. We have add the constant 1 in Eq. (29) so that the integrand reduces to zero when $G \to G_0$. Functional (28), together with the stationary condition (11) reproduce the exact Dyson's equation (25).

Coupling-Constant-Integral Form for the Generating Functional of Green's Functions

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$$Z \equiv \mathrm{tr}\left\{ T\exp\left[-\frac{i}{\hbar}\sum_{\sigma}\int_{p} d1 \int_{p} d1'\, \psi^{+}_{H\sigma}(1)\,\phi(1,1')\,\psi_{H\sigma}(1')\right] \rho \right\} \tag{1}$$

$$= \mathrm{tr}\,[S\rho]$$

$$= \sum_{mn} \rho_m \langle m|S_-|n\rangle\langle n|S_+|m\rangle \tag{2}$$

§. Incoming Interaction Picture

$$\boxed{\begin{aligned} |\psi_T(t)\rangle &= e^{iT(t+t_0)/\hbar}\,|\psi_S(t)\rangle && (3)\\ \mathcal{O}_T(t) &= e^{iT(t+t_0)/\hbar}\,\mathcal{O}_S\, e^{-iT(t+t_0)/\hbar} && (4)\end{aligned}}$$

Then,

$$|\psi_T(t)\rangle = \mathcal{J}_\pm(t,t')\,|\psi_T(t')\rangle \quad \text{according to } t \gtrless t' \tag{5}$$

where

$$\mathcal{J}_\pm(t,t') = T_\pm \exp\left\{-\frac{i}{\hbar}\int_{t'}^{t} dt_1\,[\,U_T(t_1) + V_T(t_1)\,]\right\} \tag{6}$$

temporally assume $\phi(1,1') = \phi(1)\delta(1,1')$

($\because$ The same proof as that for $S_\pm$.)

Here,

$$|\psi_H(t)\rangle = e^{iH(t+t_0)/\hbar}\,|\psi_S(t)\rangle$$

$$= e^{iH(t+t_0)/\hbar}\, e^{-iT(t+t_0)/\hbar}\,\underbrace{|\psi_T(t)\rangle}_{\mathcal{J}_\pm(t,t')\,\underbrace{|\psi_T(t')\rangle}_{\underbrace{e^{iT(t'+t_0)/\hbar}|\psi_S(t')\rangle}_{= e^{iT(t'+t_0)/\hbar} e^{-iH(t'+t_0)/\hbar}|\psi_H(t')\rangle}}}$$

$$\therefore\ \underline{S_\pm(t,t') = e^{iH(t+t_0)/\hbar}\, e^{-iT(t+t_0)/\hbar}\,\mathcal{J}_\pm(t,t')\, e^{iT(t'+t_0)/\hbar}\, e^{-iH(t'+t_0)/\hbar}} \tag{7}$$

Then, in this picture,

$$Z = \sum_{mn} \rho_m \langle m | \mathcal{T}_- | n \rangle \cancel{e^{2iTt_0/\hbar}} \cancel{e^{-2iHt_0/\hbar}}$$
$$\times \cancel{e^{2iHt_0/\hbar}} \cancel{e^{-2iTt_0/\hbar}} \langle n | \mathcal{T}_+ | m \rangle$$

$$= \mathrm{tr}\,[\mathcal{T}\rho]$$

In summary, if $\Phi(1,1') = \Phi(1)\delta_p(1,1')$,

$$Z = \mathrm{tr}\left\{ T \exp\left[-\frac{i}{\hbar}\int_p dt\, V_H(t)\right] \rho \right\} = \mathrm{tr}(S\rho) \tag{8}$$

$$= \mathrm{tr}\left\{ T \exp\left[-\frac{i}{\hbar}\int_p dt\, (U_T(t) + V_T(t))\right] \rho \right\} = \mathrm{tr}(\mathcal{T}\rho) \tag{9}$$

§. Coupling-Constant Integral

If we replace $e^2 \to \lambda$, then

$$\frac{\partial}{\partial\lambda} U = \sum_{\sigma\sigma'} \iint \frac{d^3r\, d^3r'}{|r-r'|} \psi_\sigma^+(r)\psi_{\sigma'}^+(r')\psi_{\sigma'}(r')\psi_\sigma(r) = \frac{1}{\lambda} U_\lambda \tag{10}$$

$$\therefore \frac{\partial}{\partial\lambda}\mathcal{J} = \sum_{n=0}^{\infty} \frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \int_p dt_1 \cdots \int_p dt_n \underbrace{\frac{\partial}{\partial\lambda} T\{[U_T(t_1)+V_T(t_1)]\cdots[U_T(t_n)+V_T(t_n)]\}}_{n\int_p dt_1 \int_p dt_2 \cdots \int_p dt_n T\left\{\frac{U_T(t_1)}{\lambda}[U_T(t_2)+V_T(t_2)]\cdots[U_T(t_n)+V_T(t_n)]\right\} \text{ (for } n\neq 0)}$$

$$= -\frac{i}{\hbar} T\left[\int_p dt_1 \frac{U_T(t_1)}{\lambda}\mathcal{J}\right] \tag{11}$$

$$\therefore \frac{\partial}{\partial\lambda} W$$

$$= -\frac{\hbar}{2}\frac{\partial}{\partial\lambda} \ln \operatorname{tr}(\mathcal{J}\rho)$$

$$= \cancel{-}\frac{\cancel{\hbar}}{2}\frac{1}{Z} \operatorname{tr}\left[\left(\cancel{-}\frac{i}{\cancel{\hbar}} T\int_p dt_1 \frac{U_T(t_1)}{\lambda}\mathcal{J}\right)\rho\right]$$

$$= \frac{i}{2}\left\langle \int_p dt_1 \frac{U_T(t_1)}{\lambda}\right\rangle$$

$$\boxed{\frac{\partial}{\partial\lambda} W = \frac{i}{2\lambda}\int_p dt \langle U(t)\rangle_\lambda} \tag{12}$$

where

$$\langle \mathcal{O}(t)\rangle = \operatorname{tr}\{T[\mathcal{O}_T(t)\mathcal{J}]\rho\} / \operatorname{tr}(\mathcal{J}\rho) \tag{13a}$$

$$= \operatorname{tr}\{T[\mathcal{O}_H(t)S]\rho\} / \operatorname{tr}(S\rho) \tag{13b}$$

Integrating Eq. (12) over λ,

$$\boxed{\begin{aligned} W &= W_0 + \frac{i}{2}\int_0^{e^2}\frac{d\lambda}{\lambda}\int_p dt\, \langle U(t)\rangle_\lambda && (14a)\\ &= W_0 + \frac{i}{4}\int_0^{e^2} d\lambda \int_p dt_1 \sum_{\sigma\sigma'} \iint \frac{dr_1 dr_2}{|r_1 - r_2|} \langle T[\psi_\sigma^+(1)\psi_{\sigma'}^+(2)\psi_{\sigma'}(2)\psi_\sigma(1)]\rangle_\lambda \Big|_{t_1=t_2} && (14b)\\ &= W_0 + \frac{i}{4}\int_0^{e^2}\frac{d\lambda}{\lambda}\int_p d1 \int_p d2\, v_\lambda(1,2) \sum_{\sigma\sigma'} \langle T[\psi_\sigma^+(1)\psi_{\sigma'}^+(2)\psi_{\sigma'}(2)\psi_\sigma(1)]\rangle_\lambda && (14c)\end{aligned}}$$

where $\quad v_\lambda(1,2) = (\lambda / |r_1 - r_2|)\,\delta_p(t_1 - t_2)$.

Note that,

$$\sum_{\sigma\sigma'} \langle \psi_\sigma^+(r_1)\psi_{\sigma'}^+(r_2)\psi_{\sigma'}(r_2)\psi_\sigma(r_1)\rangle$$

$$= \sum_{\sigma\sigma'} [\langle \psi_\sigma^+(r_1)\psi_\sigma(r_1)\psi_{\sigma'}^+(r_2)\psi_{\sigma'}(r_2)\rangle - \delta_{\sigma\sigma'}\delta_p(r_1 - r_2)\langle \psi_\sigma^+(r_1)\psi_\sigma(r_2)\rangle]$$

$$= \langle \rho(r_1)\rho(r_2)\rangle - \delta(r_1 - r_2)\langle \rho(r_1)\rangle$$

Then,

$$W = W_0 + \frac{i}{4}\int_0^{e^2}\frac{d\lambda}{\lambda}\int_p d1\int_p d2\, v_\lambda(1,2)\{\underbrace{\langle T[\rho(1)\overset{\langle\rho(2)\rangle + \delta\rho(2)}{\rho(2)}]\rangle_\lambda} - \delta_p(1,2)\langle\rho(1)\rangle_\lambda\}$$

$$= \langle \rho(1)\rangle\langle\rho(2)\rangle + \underbrace{\langle T[\rho(1)\delta\rho(2)]\rangle}_{i\hbar\chi(1,2)}$$

$$\boxed{\begin{aligned} \therefore\ W = W_0 &+ \frac{i}{4}\int_0^{e^2}\frac{d\lambda}{\lambda}\int_p d1\int_p d2\, v_\lambda(1,2)\,[\langle\rho(1)\rangle_\lambda\langle\rho(2)\rangle_\lambda - \delta_p(1,2)\langle\rho(1)\rangle_\lambda]\\ &- \frac{\hbar}{4}\int_0^{e^2}\frac{d\lambda}{\lambda}\int_p d1\int_p d2\, \chi(1,2)_\lambda && (15)\end{aligned}}$$

§. Comparison between LW and CCI Schemes

In Luttinger-Ward form, W is expressed as,

$$W = \Gamma + \mathcal{G}(\bar{1},\bar{1}')\Phi(\bar{1}',\bar{1})$$

$$= \underbrace{\hbar\,\mathrm{tr}\,[\ln \mathcal{G}_0^{-1}(\bar{1},\bar{1}')\mathcal{G}(\bar{1}',\bar{1}) - \mathcal{G}_0^{-1}(\bar{1},\bar{1}')\mathcal{G}(\bar{1}',\bar{1})+1] + \mathcal{G}(\bar{1},\bar{1}')\Phi(\bar{1}',\bar{1})}_{W_0}$$

$$\underbrace{-i v(\bar{1},\bar{2})\mathcal{G}(\bar{1},\bar{1}^+)\mathcal{G}(\bar{2},\bar{2}^+)}_{\frac{i}{4}v(\bar{1},\bar{2})\langle\rho(\bar{1})\rangle\langle\rho(\bar{2})\rangle} + \Xi$$

(Luttinger-Ward Form)

$$W = W_0 + \frac{i}{4}v(\bar{1},\bar{2})\langle\rho(\bar{1})\rangle\langle\rho(\bar{2})\rangle + \Xi \qquad (16)$$

where

$$\begin{cases} W_0 = \hbar\,\mathrm{tr}\,[\ln \mathcal{G}_0^{-1}\mathcal{G} - \mathcal{G}_0^{-1}\mathcal{G} + 1] + \mathrm{tr}[\mathcal{G}\Phi] & (17) \\ \mathcal{G}_0^{-1} = \left(i\frac{\partial}{\partial t_1} + \frac{\hbar}{2m}\nabla_1^2\right)\delta_p(1,1') & (18) \\ \delta\Xi/\delta\mathcal{G}(1,1') = \Sigma(1,1') & (19) \end{cases}$$

(Coupling-Constant-Integral Form)

$$W = W_0 + \frac{i}{4}\int_0^{e^2}\frac{d\lambda}{\lambda}v_\lambda(\bar{1},\bar{2})\,[\langle\rho(1)\rangle_\lambda\langle\rho(2)\rangle_\lambda - \delta_p(\bar{1},\bar{2})\langle\rho(1)\rangle_\lambda]$$

$$- \frac{\hbar}{4}\int_0^{e^2}\frac{d\lambda}{\lambda}\underbrace{\chi(\bar{1},\bar{2})_\lambda}_{v_\lambda(\bar{1},\bar{2})} \qquad (20)$$

In deriving Eq. (16), we have set $\Gamma_0 + \mathrm{tr}[\mathcal{G}\Phi] = W_0$, because in the case $U=0$ a similar derivation to that leads to W gives that form.

Field Theoretical Analysis of the Exchange-Correlation Potentials : Preliminaries

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§. Hamiltonian

$$H(t) = T + U + V(t) \tag{1}$$

$$\begin{cases} T = \sum_\sigma \int d^3r\, \psi_\sigma^\dagger(r) \left(-\frac{\hbar^2}{2m}\nabla^2\right) \psi_\sigma(r) & (2) \\ U = \frac{1}{2}\sum_{\sigma\sigma'} \int d^3r \int d^3r'\, \psi_\sigma^\dagger(r)\psi_{\sigma'}^\dagger(r')\, u(r-r')\, \psi_{\sigma'}(r')\psi_\sigma(r) & (3) \\ V(t) = \int d^3r\, \rho(r)\, v(r,t) & (4) \end{cases}$$

where $\rho(r) = \sum_\sigma \psi_\sigma^\dagger(r)\psi_\sigma(r)$.

According to Harris and Jones [J. Phys. F4, 1170 (1974)], we decompose the Hamiltonian (1) into two parts:

$$H(t) = [\, T + V_{eff}(t)\,] + [\, U + V(t) - V_{eff}(t)\,] \tag{5a}$$

$$= H_0(t) + H_1(t) \tag{5b}$$

where

$$V_{eff}(t) = \int d^3r\, \rho(r) \underbrace{\Big[\underbrace{v(r,t) + \overbrace{\int d^3r'\, u(r-r')\, n(r',t)}^{v_{ind}(r,t)}}_{v_H(r,t)} + v_{xc}(r,t) \Big]}_{v_{eff}(r,t)} \tag{6}$$

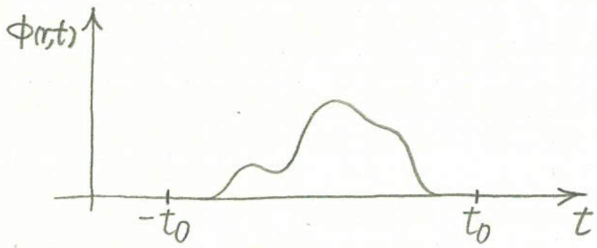
and $n(r) = \langle \Psi(t) | \rho(r) | \Psi(t) \rangle$. Equation (6) is the single-particle potential in the time-dependent Kohn-Sham formalism. As a result, the density expectation values take on the same values for both systems governed by $H_0(t)$ and $H(t)$.

According to Eq. (6),

$$H_1(t) = U - \int d^3r\, \rho(r) [\, \underbrace{v_{ind}(r,t) + v_{xc}(r,t)}_{w(r,t)} \,] \tag{7}$$

§. Generating Field

$$\begin{cases} \mathcal{H}(t) = H(t) + \Phi(t) & (8) \\ \Phi(t) = \int d^3r\, \rho(r)\, \phi(r,t) & (9) \end{cases}$$



We specify an initial state at time $-t_0$. After that an external field $\phi(r,t)$ is turned on and off before $t=t_0$.

(Schrödinger Picture)

$$|\psi_S(t)\rangle = \mathcal{U}^S_{\pm}(t,t')\,|\psi_S(t')\rangle \quad \text{according to } t \gtrless t' \tag{10}$$

where

$$\mathcal{U}^S_{\pm}(t,t') = T_{\pm} \exp\left[-\frac{i}{\hbar}\int_{t'}^{t} dt_1\, \mathcal{H}(t_1)\right] \tag{12}$$

and

① $$\mathcal{U}^S_{\pm}(t,t) = 1 \tag{13}$$

② $$i\hbar\frac{\partial}{\partial t}\mathcal{U}^S_{\pm}(t,t') = \mathcal{H}(t)\,\mathcal{U}^S_{\pm}(t,t') \tag{14a}$$

$$i\hbar\frac{\partial}{\partial t'}\mathcal{U}^S_{\pm}(t,t') = -\,\mathcal{U}^S_{\pm}(t,t')\,\mathcal{H}(t') \tag{14b}$$

③ $$\mathcal{U}^S_{\pm}(t_1,t_2)\,\mathcal{U}^S_{\pm}(t_2,t_3) = \mathcal{U}^S_{\pm}(t_1,t_3) \tag{15}$$

with signs $\pm$ according to $t_{left} \gtrless t_{right}$

④ $$\mathcal{U}^S_{\pm}(t,t')^{-1} = \mathcal{U}^S_{\pm}(t,t')^{\dagger} = \mathcal{U}^S_{\mp}(t',t) \tag{16}$$

(Heisenberg Picture)

$$\begin{cases} |\Psi_0\rangle = |\Psi_S(-t_0)\rangle & (17) \\ \mathcal{O}_0(t) = \mathcal{U}_-^S(-t_0, t)\, \mathcal{O}_S\, \mathcal{U}_+^S(t, -t_0) & (18) \end{cases}$$

then

$$\langle \Psi_S(t_1)|\, \mathcal{O}_S\, \mathcal{U}_\pm^S(t_1, t_2)\, \mathcal{O}_S\, |\Psi_S(t_2)\rangle = \langle \Psi_0|\, \mathcal{O}_0(t_1)\, \mathcal{O}_0(t_2)\, |\Psi_0\rangle \qquad (19)$$

(Interaction Picture)

$$\begin{cases} |\Psi_H(t)\rangle \equiv \mathcal{U}_-^H(-t_0, t)\, |\Psi_S(t)\rangle & (20) \\ \mathcal{O}_H(t) \equiv \mathcal{U}_-^H(-t_0, t)\, \mathcal{O}_S\, \mathcal{U}_+^H(t, -t_0) & (21) \end{cases}$$

where

$$\mathcal{U}_\pm^H(t, t') = T_\pm \exp\left[-\frac{i}{\hbar}\int_{t'}^{t} dt_1\, H(t_1)\right] \qquad (22)$$

Then,

$$i\hbar\frac{\partial}{\partial t}|\Psi_H(t)\rangle = \underbrace{\left[i\hbar\frac{\partial}{\partial t}\mathcal{U}_-^H(-t_0, t)\right]}_{-\mathcal{U}_-^H(-t_0,t)\, H(t)\ \text{[cf. Eq. (14b)]}}|\Psi_S(t)\rangle + \mathcal{U}_-^H(-t_0, t)\underbrace{\left[i\hbar\frac{\partial}{\partial t}|\Psi_S(t)\rangle\right]}_{\mathcal{H}(t)\,|\Psi_S(t)\rangle}$$

$$= \mathcal{U}_-^H(-t_0, t)\left[\mathcal{H}(t) - H(t)\right]\underbrace{\ \ }_{\mathcal{U}_+^H(t,-t_0)\,\mathcal{U}_-^H(-t_0,t)}|\Psi_S(t)\rangle$$

$$= \Phi_H(t)\, |\Psi_H(t)\rangle$$

$$\therefore\ i\hbar\frac{\partial}{\partial t}|\Psi_H(t)\rangle = \Phi_H(t)\, |\Psi_H(t)\rangle \qquad (23)$$

so that

$$\begin{cases} |\Psi_H(t)\rangle = S_\pm(t, t')\, |\Psi_H(t')\rangle \quad \text{according to } t \gtrless t' & (24) \\ S_\pm(t, t') = T_\pm \exp\left[-\frac{i}{\hbar}\int_{t'}^{t} dt_1\, \Phi_H(t_1)\right] & (25) \end{cases}$$

① $S_\pm(t_1,t_2)S_\pm(t_2,t_3) = S_\pm(t_1,t_3)$ with signs $\pm$ according to $t_{\text{left}} \gtrless t_{\text{right}}$ (26)

② $S_\pm^{-1}(t,t') = S_\pm^\dagger(t,t') = S_\mp(t',t)$ (27)

③ $\langle\Psi_0|\,\mathcal{O}_0(t_1)\mathcal{O}_0(t_2)\,|\Psi_0\rangle$

$= \langle\Psi_0|\,S_-(-\infty,t_1)\mathcal{O}_H(t_1)S_\pm(t_1,t_2)\mathcal{O}_H(t_2)S_+(t_2,-\infty)\,|\Psi_0\rangle$ (28)

∵③

(i) $|\Psi_S(t)\rangle = \mathcal{U}^H_+(t,-t_0)\,|\Psi_H(t)\rangle$

$$= \underbrace{\mathcal{U}^H_+(t,-t_0)\,S_\pm(t,t')\,\mathcal{U}^H_-(-t_0,t)}_{=\mathcal{U}^S_\pm(t,t')}\,|\Psi_S(t')\rangle$$

In particular setting $t'=-t_0$,

$$|\Psi_S(t)\rangle = \mathcal{U}^H_+(t,-t_0)\,S_+(t,-\infty)\,|\Psi_0\rangle$$

(ii) $\langle\Psi_S(t_1)|\,\mathcal{O}_S\,\mathcal{U}_\pm(t_1,t_2)\,\mathcal{O}_S\,|\Psi_S(t_2)\rangle$

$$= \langle\Psi_0|S_-(-\infty,t_1)\underbrace{\mathcal{U}^H_-(-t_0,t_1)\,\mathcal{O}_S\,\mathcal{U}^H_+(t_1,-t_0)}_{\mathcal{O}_H(t_1)}S_\pm(t_1,t_2)\underbrace{\mathcal{U}^H_-(-t_0,t_2)\,\mathcal{O}_S\,\mathcal{U}^H_+(t_2,-t_0)}_{\mathcal{O}_H(t_2)}S_+(t,-\infty)|\Psi_0\rangle$$

//

§. Response Theorem

$$\frac{\delta S_\pm(t,t')}{\delta\phi(1)} = \mp\frac{i}{\hbar}\Theta_\pm(t,t_1,t')\,T_\pm[\rho_H(1)S_\pm(t,t_0)]$$ (29)

where

$\Theta_+(t_1,\dots,t_n) = \theta(t_1-t_2)\cdots\theta(t_{n-1}-t_n)$ (30a)

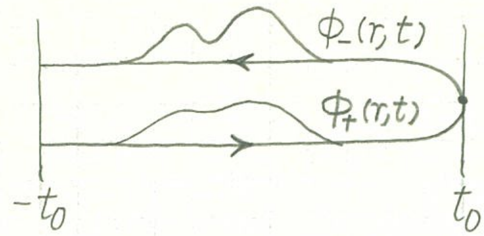
$\Theta_-(t_1,\dots,t_n) = \theta(t_n-t_{n-1})\cdots\theta(t_2-t_1)$ (30b)

∵ Functional derivative is defined so that

$$\delta f = \int_{-\infty}^{\infty}dt\,\frac{\delta f}{\delta g(t)}\,\delta g(t) = -\int_{\infty}^{-\infty}dt\,\frac{\delta f}{\delta g(t)}\,\delta g(t)$$

//

§. Closed Time Path



$$S = T \exp\left[-\frac{i}{\hbar}\int d^3r \int_P dt\, \rho_H(r,t)\,\phi(r,t)\right] \tag{31a}$$

$$\equiv T_- \exp\left[-\frac{i}{\hbar}\int d^3r \int_{\infty}^{-\infty} dt\, \rho_H(r,t)\,\phi_-(r,t)\right] T_+ \exp\left[-\frac{i}{\hbar}\int d^3r \int_{-\infty}^{\infty} dt\, \rho_H(r,t)\,\phi_+(r,t)\right] \tag{31b}$$

$$= S_- S_+ \tag{31c}$$

① $$\begin{cases} i\hbar\frac{\partial}{\partial t} S(t,t') = \Phi_H(t)\, S(t,t') & (32a) \\ i\hbar\frac{\partial}{\partial t'} S(t,t') = -S(t,t')\,\Phi_H(t') & (32b) \end{cases}$$

② $$\frac{\delta S(t,t')}{\delta \phi(1)} = -\frac{i}{\hbar}\Theta(t,t_1,t')\, T[\rho_H(1) S(t,t')] \tag{33}$$

where $\Theta(t,t_1,t') = 1$ for $t \gtrsim_p t_1 \gtrsim_p t'$ and $=0$ otherwise; $t \gtrsim_p t_1$ means that t is later than t_1 on the closed time path.

∵ ②

$$\delta f = \int_P \frac{\delta f}{\delta g(t)}\, \delta g(t)\, dt$$

$$= \int_{-\infty}^{\infty} \frac{\delta f}{\delta g(t)}\, \delta g(t)\, dt + \int_{\infty}^{-\infty} \frac{\delta f}{\delta g(t)}\, \delta g(t)\, dt$$

Therefore, there is no additional minus sign in contrast to the case of Eq. (29).

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§. Nonlocal S Matrix

$$S \equiv T \exp\left[-\frac{i}{\hbar}\sum_\sigma \int_P d1 \int_P d1' \, \psi^+_{H\sigma}(1)\,\phi(1,1')\,\psi_{H\sigma}(1')\right] \tag{1}$$

(Response Theorem)

$$\text{(A)}\quad \frac{\delta S}{\delta\phi(1,1')} = -\frac{i}{\hbar}\sum_\sigma \left[\psi^+_{H\sigma}(1)\psi_{H\sigma}(1')S\right] \tag{2}$$

$$\text{(B)}\quad \frac{\delta\langle T[A(t)B(t')\cdots]\rangle}{\delta\phi(1,1')} = -\frac{i}{\hbar}\sum_\sigma \langle T\{\delta[\psi^+_\sigma(1)\psi_\sigma(1')]A(t)B(t')\cdots\}\rangle \tag{3}$$

where

$$\delta[\psi^+_\sigma(1)\psi_\sigma(1')] = \psi^+_\sigma(1)\psi_\sigma(1') - \langle\psi^+_\sigma(1)\psi_\sigma(1')\rangle \tag{4}$$

$$\langle\theta(t)\rangle = \mathrm{tr}\{T[\theta_H(t)S]\rho\} / \mathrm{tr}(S\rho) \tag{5}$$

(Response Functions)

$$\chi^{(\nu)}(1,1';\ldots;\nu,\nu') = \frac{\delta^{\nu-1}}{\delta\phi(\nu,\nu')\cdots\delta\phi(2,2')}\sum_\sigma\langle T[\psi^+_\sigma(1)\psi_\sigma(1')]\rangle \tag{6}$$

In particular,

$$\chi(1,2) = \chi^{(2)}(1^+,1;2^+,2) \tag{7}$$

is the density response function, where $1^+ = (r_1, t_1 + 0_P)$, and 0_P means an infinitesimal later time on the closed time path.

§. Generating Functional

$$Z \equiv \mathrm{tr}(S\rho) \tag{8}$$

$$W \equiv -\frac{\hbar}{2}\ln Z \tag{9}$$

Then,

$$\frac{\delta W}{\delta \Phi(1',1)} = \mathcal{G}(1,1') \tag{10}$$

where the single-particle Green's function is defined as

$$\mathcal{G}(1,1') = -\frac{i}{2}\sum_{\sigma}\langle T[\psi_\sigma(1)\psi^\dagger_\sigma(1')]\rangle \tag{11}$$

§. Vertex Functional

By performing the Legendre transform, we define the vertex functional Γ as

$$\Gamma[\mathcal{G}(1,1')] \equiv W[\Phi(1,1')] - \int_P d1\int_P d1'\, \mathcal{G}(1,1')\Phi(1',1) \tag{12a}$$

$$\equiv W - \mathrm{tr}(\mathcal{G}\Phi) \tag{12b}$$

Then, using Eq. (10),

$$\frac{\delta \Gamma}{\delta \mathcal{G}(1,1')} = -\Phi(1',1) \tag{13}$$

We define the ν-body vertex functions $\Gamma^{(\nu)}$ as the functional derivatives of Γ with respect to Green's functions,

$$\Gamma^{(\nu)}(1,1',\dots,\nu,\nu') \equiv \frac{\delta^\nu}{\delta\mathcal{G}(\nu,\nu')\cdots\delta\mathcal{G}(1,1')}\Gamma \tag{14}$$

§. Equation of Motion for the Green's Function

$$i\frac{\partial}{\partial t_1} g(1,1') - \frac{1}{\hbar}\int_p d2\,\Phi(1,2)\,g(2,1') + \frac{i}{2\hbar}\sum_\sigma \langle T\{[\psi_\sigma(1), H(t_1)]\,\psi_\sigma^+(1')\}\rangle$$
$$= \delta_p(1,1') \qquad (8)$$

where

$$\delta_p(t-t') = \frac{d}{dt}\Theta_p(t-t') = \begin{cases} \delta(t-t') & \text{for } (t,t')\in(+,+) \\ -\delta(t-t') & \phantom{\text{for }}(-,-) \\ 0 & \text{otherwise} \end{cases} \qquad (9)$$

① $$[\psi_\sigma(r), H_0(t)] = \sum_\lambda \int d^3x\, [\psi_\sigma(r), \psi_\lambda^+(x)(-\frac{\hbar^2}{2m}\nabla^2 + v_{\text{eff}}(x,t))\psi_\lambda(x)]$$
$$= \underline{(-\frac{\hbar^2}{2m}\nabla^2 + v_{\text{eff}}(r,t))\,\psi_\sigma(r)}$$

② $$[\psi_\sigma(r), H_1(t)] = [\psi_\sigma(r), U - \int d^3x\,\rho(x)\,w(x,t)]$$
$$= \frac{1}{2}\sum_{\lambda\lambda'}\int d^3x \int d^3x'\, u(x-x')\,[\psi_\sigma(r), \psi_\lambda^+(x)\psi_{\lambda'}^+(x')\psi_{\lambda'}(x')\psi_\lambda(x)] - w(r,t)\,\psi_\sigma(r)$$
$$= \underline{\int d^3x\, u(r-x)\,\rho(x)\,\psi_\sigma(r) - w(r,t)\,\psi_\sigma(r)}$$

$$\therefore\ [i\frac{\partial}{\partial t_1} + \frac{\hbar}{2m}\nabla_1^2 - \frac{1}{\hbar}v_{\text{eff}}(1)]\,g(1,1') - \frac{1}{\hbar}\Phi(1,\bar{2})\,g(\bar{2},1')$$
$$+ \frac{i}{2\hbar}\sum_\sigma \underbrace{\int d^3x\, u(r-x)\,\langle T[\rho(x,t_1)\psi_\sigma(1)\psi_\sigma^+(1')]}\rangle + \frac{1}{\hbar}w(1)\,g(1,1')$$
$$\frac{i}{2\hbar}\sum_\sigma u(1^+,\bar{2})\langle T[\underbrace{\rho(\bar{2})}_{n(\bar{2})+\delta\rho(\bar{2})}\psi_\sigma(1)\psi_\sigma^+(1')]\rangle \qquad = \delta_p(1,1')$$

$$= -\frac{i}{2\hbar}\sum_\sigma u(1^+,\bar{2})\langle T[\delta\rho(\bar{2})\psi_\sigma^+(1')\psi_\sigma(1)]\rangle - \frac{1}{\hbar}\underbrace{u(1^+\bar{2})\,n(\bar{2})}_{v_{ind}(1)}g(1,1')$$

$$= \frac{1}{2}u(1^+,\bar{2})\,\chi^{(2)}(1',1;\bar{2}^+,\bar{2}) - \frac{1}{\hbar}v_{ind}(1)\,g(1,1')$$

$$[i\frac{\partial}{\partial t_1}+\frac{\hbar}{2m}\nabla_1^2-\frac{1}{\hbar}v_{eff}(1)]\,\mathcal{G}(1,1')-\frac{1}{\hbar}\Phi(1,\bar{2})\mathcal{G}(\bar{2},1')$$
$$+\frac{1}{2}\mathcal{U}(1^+,\bar{2})\,\chi^{(2)}(1',1;\bar{2}^+,\bar{2})+\frac{1}{\hbar}\underbrace{[w(1)-v_{ind}(1)]}_{v_{xc}(1)}\mathcal{G}(1,1')\;=\;\delta_p(1,1')$$

$$\boxed{\begin{aligned}&[i\frac{\partial}{\partial t_1}+\frac{\hbar}{2m}\nabla_1^2-\frac{1}{\hbar}v_{eff}(1)]\,\mathcal{G}(1,1')-\frac{1}{\hbar}\Phi(1,\bar{2})\mathcal{G}(\bar{2},1')\\&\quad+\frac{1}{2}\mathcal{U}(1^+,\bar{2})\chi^{(2)}(1',1;\bar{2}^+,\bar{2})+\frac{1}{\hbar}v_{xc}(1)\mathcal{G}(1,1')\;=\;\delta_p(1,1')\end{aligned}} \qquad (10)$$

(Dyson Equation)

Introducing the self-energy as

$$\Sigma(1,1')\;=\;-\frac{1}{2}\mathcal{U}(1^+,\bar{2})\chi^{(2)}(\bar{3},1;\bar{2}^+,\bar{2})\mathcal{G}^{-1}(\bar{3},1')-\frac{1}{\hbar}v_{xc}(1)\delta_p(1,1') \qquad (11a)$$

$$\equiv\;\Sigma_{xc}(1,1')\;-\;\frac{1}{\hbar}v_{xc}(1)\,\delta_p(1,1')\,, \qquad (11b)$$

Equation (10) can be rewritten as

$$[i\frac{\partial}{\partial t_1}+\frac{\hbar}{2m}\nabla_1^2-\frac{1}{\hbar}v_{eff}(1)]\,\delta_p(1,\bar{2})\mathcal{G}(\bar{2},1')\;-\frac{1}{\hbar}\Phi(1,\bar{2})\mathcal{G}(\bar{2},1')$$
$$-\;\Sigma(1,\bar{2})\,\mathcal{G}(\bar{2},1')\;=\;\delta_p(1,1') \qquad (12)$$

or

$$\mathcal{G}^{-1}(1,1')\;=\;\mathcal{G}_0^{-1}(1,1')-\frac{1}{\hbar}\Phi(1,1')-\Sigma(1,1') \qquad (13)$$

where

$$\mathcal{G}_0^{-1}(1,1')\;=\;[i\frac{\partial}{\partial t_1}+\frac{\hbar}{2m}\nabla_1^2-\frac{1}{\hbar}v_{eff}(1)]\,\delta_p(1,1') \qquad (14)$$

Comparing Eq. (13) with Eq. (13),

$$\frac{\delta\Gamma}{\delta\mathcal{G}(1,1')} = \hbar\,\mathcal{G}^{-1}(1',1) - \hbar\,\mathcal{G}_0^{-1}(1',1) + \hbar\,\Sigma(1',1) \tag{15}$$

$$\therefore\ \delta\Gamma = \hbar\,[\underbrace{\mathcal{G}^{-1}(\bar{1}',\bar{1})\delta\mathcal{G}(\bar{1}\bar{1}')}_{=-\mathcal{G}(\bar{1},\bar{1}')\delta\mathcal{G}^{-1}(\bar{1}',\bar{1})} - \mathcal{G}_0^{-1}(\bar{1}',\bar{1})\delta\mathcal{G}(\bar{1},\bar{1}') + \Sigma(\bar{1}',\bar{1})\delta\mathcal{G}(\bar{1},\bar{1}')]$$

$$(\because\ \delta(\mathcal{G}\mathcal{G}^{-1}) = (\delta\mathcal{G})\mathcal{G}^{-1} + \mathcal{G}\,\delta\mathcal{G}^{-1} = 0\ )$$

$$= -\hbar\,\mathrm{tr}\,(\mathcal{G}\,\delta\mathcal{G}^{-1} + \mathcal{G}_0^{-1}\delta\mathcal{G} - \Sigma\,\delta\mathcal{G}\ )$$

$$\boxed{\begin{array}{lll} \Gamma = -\hbar\,\mathrm{tr}\,[\ln\mathcal{G}^{-1} + \mathcal{G}_0^{-1}\mathcal{G} - 1] + \hbar\,\Xi' & & (16) \\ \text{where} & & \\ \delta\,\mathrm{tr}\,(\ln\mathcal{G}^{-1}) = \mathcal{G}(\bar{1},\bar{1}')\delta\mathcal{G}(\bar{1}',\bar{1}) & & (17) \\ \mathrm{tr}\,(\mathcal{G}_0^{-1}\mathcal{G}\ ) = \mathcal{G}_0^{-1}(\bar{1},\bar{1}')\mathcal{G}(\bar{1}',\bar{1}) & & (18) \\ \delta\Xi'/\delta\mathcal{G}(1,1') \equiv \Sigma(1,1') & & (19) \end{array}}$$

§. Generator

From Eqs. (12) and (16),

$$W = \Gamma + \mathrm{tr}\,\mathcal{G}\Phi$$

$$= -\hbar\,\mathrm{tr}\,[\ln\mathcal{G}^{-1} + \underbrace{\mathcal{G}_0^{-1}\mathcal{G} - \tfrac{1}{\hbar}\Phi\mathcal{G}}_{(\mathcal{G}_0^{-1}-\frac{1}{\hbar}\Phi)\mathcal{G}} - 1] + \hbar\,\Xi'$$

$$= (\mathcal{G}^{-1}+\Sigma)\mathcal{G} = 1 + \Sigma\mathcal{G}\quad (\because\ \text{Eq. (13)}\ )$$

$$= -\hbar\,\mathrm{tr}\,[\ln\mathcal{G}^{-1} + \Sigma\mathcal{G}] + \hbar\,\Xi'$$

$$\boxed{W = -\hbar\, \mathrm{tr}[\ln \mathcal{G}^{-1} + \Sigma \mathcal{G}] + \hbar \Xi'} \qquad (20)$$

In the same way, for the system $H_1 \to 0$,

$$W_0 = -\hbar\, \mathrm{tr}[\ln \mathcal{G}_0^{-1}] \qquad (21)$$

Introducing Ξ by

$$\delta \Xi / \delta \mathcal{G}(1,1') = \Sigma_{xc}(1,1') \qquad (22)$$

$$\therefore\ W - W_0 = -\hbar\, \mathrm{tr}[\ln \underbrace{(\mathcal{G}^{-1}/\mathcal{G}_0^{-1})} + \Sigma \mathcal{G}] + \hbar \Xi + \frac{i}{2} v_{xc}(\bar{1}) n(\bar{1})$$

$$\frac{\mathcal{G}_0^{-1} - \Sigma}{\mathcal{G}_0^{-1}} = 1 - \mathcal{G}_0 \Sigma \ ?$$

$$W = W_0 - \hbar\, \mathrm{tr}[\ln(1 - \Sigma \mathcal{G}_0) + \Sigma \mathcal{G}] + \frac{i}{2} v_{xc} n + \hbar \Xi \qquad (23)$$

where

$$\delta \Xi / \delta \mathcal{G}(1,1') = \Sigma_{xc}(1,1') \qquad (24)$$

Suppose that $v_{eff}(1)$ and $w(1)$ are external sources, then

$$\mathcal{G}^{-1}(1,1') = \mathcal{G}_0^{-1}(1,1') - \tfrac{1}{\hbar}\phi(1,1') + \tfrac{1}{\hbar}w(1)\delta_p(1,1') - \tfrac{1}{\hbar}v_{ind}(1)\delta_p(1,1') - \Sigma_{xc}(1,1')$$

$$\frac{\delta\Gamma}{\delta\mathcal{G}(1,1')} = \hbar\mathcal{G}^{-1}(1',1) - \hbar\mathcal{G}_0^{-1}(1',1) - w(1)\delta_p(1,1') + u(1,\bar{2})n(\bar{2})\delta_p(1,1') + \hbar\Sigma_{xc}(1,1')$$

$$\boxed{\Gamma = -\hbar[\mathrm{tr}\ln\mathcal{G}^{-1} + \mathcal{G}_0^{-1}\mathcal{G} - 1] - \tfrac{i}{2}wn + \tfrac{i}{4}unn + \hbar\Xi} \qquad (1')$$

where

$$\boxed{\delta\Xi/\delta\mathcal{G}(1,1') = \Sigma_{xc}(1,1')} \qquad (2')$$

$$W = \Gamma + \hbar\,\mathrm{tr}\,\mathcal{G}\phi$$

$$= -\hbar\,\mathrm{tr}[\ln\mathcal{G}^{-1} + \underbrace{(\mathcal{G}_0^{-1} - \tfrac{1}{\hbar}\phi)\mathcal{G}}_{(\mathcal{G}^{-1}+\Sigma)\mathcal{G} = \cancel{1} + \Sigma\mathcal{G}} - \cancel{1}] \underbrace{- \tfrac{i}{2}wn + \tfrac{i}{4}unn}_{} + \Xi$$

$$-\tfrac{i}{2}(un + v_{xc})n + \tfrac{i}{4}unn$$

$$= -\tfrac{i}{4}unn - \tfrac{i}{2}v_{xc}n$$

$$W = -\hbar\,\mathrm{tr}[\ln\mathcal{G}^{-1} + \Sigma\mathcal{G}] - \tfrac{i}{4}unn - \tfrac{i}{2}v_{xc}n + \hbar\Xi \qquad (3')$$

Since

$$W_0 = -\hbar\,\mathrm{tr}(\ln\mathcal{G}_0^{-1}) \qquad (4')$$

$$\boxed{W - W_0 = -\hbar\,\mathrm{tr}[\ln(1 - \Sigma\mathcal{G}_0) + \Sigma\mathcal{G}] - \tfrac{i}{4}unn - \tfrac{i}{2}v_{xc}n + \hbar\Xi} \qquad (5')$$

§. Sham Equation [Sham, Phys. Rev. B32, 3876 (1985)]

Multiplying Eq. (13) by $\mathcal{G}_0 \times (\cdots) \times \mathcal{G}$,

$$\mathcal{G}_0(1,1') = \mathcal{G}(1,1') - \frac{1}{\hbar}\mathcal{G}_0(1,\bar{2})\phi(\bar{2},\bar{3})\mathcal{G}(\bar{3},\bar{1}') - \mathcal{G}_0(1,\bar{2})\Sigma(\bar{2},\bar{3})\mathcal{G}(\bar{3},1')$$

Considering a physical system in which $\phi = 0$,

$$\boxed{\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 \Sigma \mathcal{G}} \qquad (15)$$

$$\mathcal{G}(1,1^+) = -\frac{i}{2}\sum_\sigma \langle T[\psi_\sigma(1)\psi_\sigma^\dagger(1')]\rangle = \frac{i}{2}n(1)$$

Since the density $n(1)$ is the same for both systems $H_0(t)$ and $H(t)$, from Eq. (15),

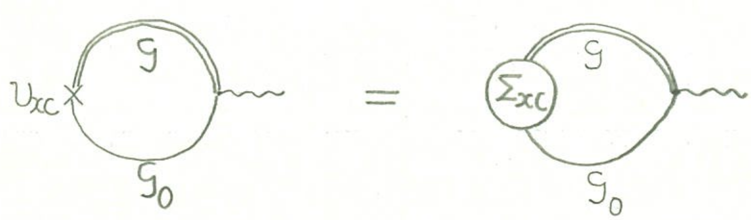
$$\boxed{\mathcal{G}_0(1,\bar{2})\Sigma(\bar{2},\bar{3})\mathcal{G}(\bar{3},1^+) = 0} \qquad (16)$$

Substituting Eq. (11) in Eq. (16),

$$\mathcal{G}_0(1,\bar{2})\left\{\Sigma_{xc}(\bar{2},\bar{3}) - \frac{1}{\hbar}v_{xc}(\bar{2})\delta_p(\bar{2},\bar{3})\right\}\mathcal{G}(\bar{3},1^+) = 0$$

$$\mathcal{G}_0(1,\bar{2})\Sigma_{xc}(\bar{2},\bar{3})\mathcal{G}(\bar{3},1^+) - \frac{1}{\hbar}\mathcal{G}_0(1,\bar{2})v_{xc}(\bar{2})\mathcal{G}(\bar{2},1^+) = 0$$

$$\boxed{\mathcal{G}_0(1,\bar{2})v_{xc}(\bar{2})\mathcal{G}(\bar{2},1^+) = \hbar\,\mathcal{G}_0(1,\bar{2})\Sigma_{xc}(\bar{2},\bar{3})\mathcal{G}(\bar{3},1^+)} \qquad (17)$$

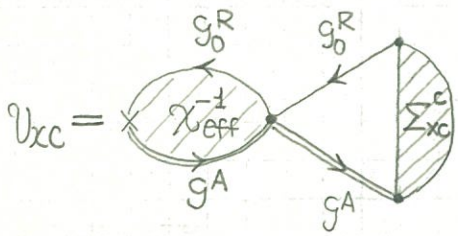


Or, defining

$$\boxed{\chi_{eff}(1,2) \equiv -\frac{2i}{\hbar}\, \mathcal{G}_0(1,2)\,\mathcal{G}(2,1) \qquad (18)}$$

$$\frac{i\cancel{\hbar}}{2}\chi_{eff}(1,\bar{2})\, v_{xc}(\bar{2}) = \cancel{\hbar}\, \mathcal{G}_0(1,\bar{2})\,\Sigma_{xc}(\bar{2},\bar{3})\,\mathcal{G}(\bar{3},1^+)$$

$$\boxed{v_{xc}(1) = -2i\, \chi_{eff}^{-1}(1,\bar{2})\,\mathcal{G}_0(\bar{2},\bar{3})\,\Sigma_{xc}(\bar{3},\bar{4})\,\mathcal{G}(\bar{4},\bar{2}^+) \qquad (19)}$$



Field-Theoretical Analysis of the xc Potential: Correlation-Function Expression 1989.9.29

Here, we assume the generating field $\phi(1,1') = \phi(1)\delta_p(1,1')$, then

$$Z = \mathrm{tr}\{ T\exp[-\frac{i}{\hbar}\int_p d1\, \rho(1)\phi(1)]\, \hat{\rho} \} \tag{1}$$

$\hookrightarrow$ density matrix

$$= \mathrm{tr}[S\hat{\rho}]$$

$$= \sum_{mn} \hat{\rho}_{mn} \langle m|S_-|n\rangle\langle n|S_+|m\rangle \tag{2}$$

§. Incoming Interaction Picture

$$|\psi_{H_0}(t)\rangle \equiv \mathcal{U}_-^{H_0}(-t_0,t)\, |\psi_S(t)\rangle \tag{3}$$

$$\mathcal{O}_{H_0}(t) \equiv \mathcal{U}_-^{H_0}(-t_0,t)\, \mathcal{O}_S\, \mathcal{U}_+^{H_0}(t,-t_0) \tag{4}$$

Then,

$$|\psi_{H_0}(t)\rangle = \mathcal{U}_\pm^{H_0}(t,t')\, |\psi_{H_0}(t')\rangle \text{ according to } t \gtrless t' \tag{5}$$

where

$$\mathcal{U}_\pm^{H_0}(t,t') = T_\pm \exp\{-\frac{i}{\hbar}\int_{t'}^{t} dt_1\, [H_{1H_0}(t_1) + \Phi_{H_0}(t_1)]\} \tag{6}$$

and

$$Z = \mathrm{tr}\{T\exp[-\frac{i}{\hbar}\int_p dt\, \Phi_H(t)]\, \hat{\rho}\} = \mathrm{tr}(S\hat{\rho}) \tag{7}$$

$$= \mathrm{tr}\{T\exp[-\frac{i}{\hbar}\int_p dt\, (H_{1H_0}(t) + \Phi_{H_0}(t))]\, \hat{\rho}\} = \mathrm{tr}(\mathcal{U}^{H_0}\hat{\rho}) \tag{8}$$

§. Coupling-Constant Integral

If we replace $H_1(t) \longrightarrow \lambda H_1(t) = H_1^\lambda(t)$, then

$$\frac{d}{d\lambda}\mathcal{U}^{H_0} = -\frac{i}{\hbar} T\left[\int_P dt \, \frac{H^\lambda_{1\,H_0}(t)}{\lambda} \mathcal{U}^{H_0}\right] \tag{9}$$

$$\therefore \frac{d}{d\lambda} W = -\frac{\hbar}{2} \, \mathrm{tr}\left(\frac{d\mathcal{U}^{H_0}}{d\lambda}\hat{\rho}\right) / \mathrm{tr}\,(\mathcal{U}^{H_0}\rho)$$

$$= \frac{i}{2}\left\langle \int_P dt_1 \frac{H^\lambda_{1\,H_0}(t)}{\lambda} \right\rangle$$

$$\therefore W = W_{\lambda=0} + \frac{i}{2}\int_0^1 d\lambda \int_P dt \, \langle H_1(t) \rangle_\lambda \tag{10}$$

where

$$\langle \vartheta(t) \rangle = \mathrm{tr}\{T[\vartheta_{H_0}(t)\,\mathcal{U}^{H_0}]\,\hat{\rho}\} / \mathrm{tr}\,(\mathcal{U}^{H_0}\hat{\rho}) \tag{11a}$$

$$= \mathrm{tr}\{T[\vartheta_H(t)\,S]\,\hat{\rho}\} / \mathrm{tr}\,(S\hat{\rho}) \tag{11b}$$

Here,

$$H_1^{\lambda}(t) = \frac{\lambda}{2}\sum_{\sigma\sigma'}\int d^3r_1\int d^3r_2\, u(r_1-r_2)\,\langle \psi_\sigma^\dagger(r_1)\psi_{\sigma'}^\dagger(r_2)\psi_{\sigma'}(r_2)\psi_\sigma(r_1)\rangle_t$$

$$-\int d^3r\, n_\lambda(r)\, w(r,t)$$

$$= \frac{\lambda}{2}\int d^3r_1\int d^3r_2\, u(r_1-r_2)\,\left[\langle\rho(r_1)\rho(r_2)\rangle_\lambda - \delta(r_1-r_2)\, n_\lambda(r_1)\right]$$

$$-\lambda\int d^3r\, n_\lambda(r)\, w(rt)$$

$$\therefore\ W = W_{\lambda=0} + \frac{i}{4}\int_0^1 d\lambda\int_p d1\int_p d2\, u(1,2)\left\{\underbrace{\langle T[\rho(1)\overbrace{\rho(2)}^{n_\lambda(2)+\delta\rho(2)}]\rangle_\lambda}_{n_\lambda(1)n_\lambda(2)+\underbrace{\langle T[\rho(1)\delta\rho(2)]\rangle_\lambda}_{i\hbar\chi_\lambda(1,2)}} - \delta_p(1,2)\, n_\lambda(1)\right\}$$

$$-\frac{i}{2}\int_0^1 d\lambda\int_p d1\, n_\lambda(1)\, w(1)$$

$$\boxed{\begin{aligned} W = W_{\lambda=0} &+ \frac{i}{4}\int_0^1 d\lambda\int_p d1\int_p d2\, u(1,2)\left[n_\lambda(1)n_\lambda(2) - \underset{?}{\cancel{\delta_p(1,2)\, n_\lambda(1)}}\right] \\ &- \frac{i}{2}\int_0^1 d\lambda\int_p d1\, n_\lambda(1)\, w(1) \\ &- \frac{\hbar}{4}\int_0^1 d\lambda\int_p d1\int_p d2\, \chi_\lambda(1,2) \qquad (12)\end{aligned}}$$

where $u(1,2) = (e^2/|r_1-r_2|)\,\delta_p(t_1-t_2)$.

Exchange-Correlation Potential in the Time-Dependent Density-Functional Theory 1989. 9. 29

§. Effective Action

$$A \equiv \int_{t_0}^{t_1} dt \, \langle \Psi(t) | i\hbar \partial/\partial t - H(t) | \Psi(t) \rangle \tag{1}$$

Here,

$$H(t) = T + U + V(t) \tag{2}$$

$$= [\underbrace{T + V_{eff}(t)}_{H_0(t)}] + [\underbrace{U + V(t) - V_{eff}(t)}_{H_1(t)}] \tag{3}$$

where

$$V_{eff}(t) = \int d^3r \, \rho(r) \, [\underbrace{\underbrace{v(r,t) + \underbrace{\int d^3r' \, \mathcal{U}(r-r') n(r',t)}_{v_{ind}(r,t)}}_{v_H(r,t)} + v_{xc}(r,t)}_{v_{eff}(r,t)}] \tag{4}$$

is the single-particle potential in the time-dependent Kohn-Sham scheme. This choice of $v_{eff}(r,t)$ makes the density expectation value $n(r,t) = \langle \rho(r,t) \rangle$ the same for both systems governed by $H_0(t)$ and $H(t)$.

According to Eq. (4),

$$H_1(t) = U - \int d^3r \, \rho(r) \, [\underbrace{v_{ind}(r,t) + v_{xc}(r,t)}_{w(r,t)}] \tag{5}$$

§ Coupling-Constant Integral

We introduce a dimensionless coupling constant such that

$$H(t) = H_0(t) + \lambda H_1(t) \tag{6}$$

Then,

$$\frac{dA}{d\lambda} = \int_{t_0}^{t_1} dt \left\{ \left\{ \frac{d}{d\lambda} \langle \psi(t) | \right\} [i\hbar \partial/\partial t - H(t)] | \psi(t) \rangle - \langle \psi(t) | H_1(t) | \psi(t) \rangle \right.$$
$$\left. + \langle \psi(t) | [i\hbar \partial/\partial t - H(t)] \frac{d}{d\lambda} | \psi(t) \rangle \right\}$$

Since we are constructing the mapping,

$$v(r,t) \longmapsto |\psi(t)\rangle \tag{7}$$

where

$$[i\hbar \partial/\partial t - H(t)] |\psi(t)\rangle = 0 \tag{8}$$

($\because$ $A = 0$ for all the cases.), we can rewrite $dA/d\lambda$ using Eq. (8) as

$$\frac{dA}{d\lambda} = \int_{t_0}^{t_1} dt \left[\underbrace{\langle i\hbar \tfrac{\partial}{\partial t} - H(t) \rangle}_{=0} \underbrace{\frac{d}{d\lambda} \langle \psi(t) | \psi(t) \rangle}_{=0} - \langle \psi(t) | H_1(t) | \psi(t) \rangle_\lambda \right]$$

$$\boxed{A = A_{\lambda=0} - \int_0^1 d\lambda \int_{t_0}^{t_1} dt \, \langle H_1(t) \rangle_\lambda} \tag{9}$$

$$\boxed{\therefore A - A_{\lambda=0} = 2i \left(W - W_{\lambda=0} \right)} \tag{10}$$

㊟ + path のみ；従って A は $v_+(r,t)$ のみに依存する.

$$\boxed{\begin{aligned} \therefore\ A - A_{\lambda=0} &= -\frac{1}{2}\int_0^1 d\lambda \int_P d1 \int_P d2\, \mathcal{U}(1,2)\, n_\lambda(1)\, n_\lambda(2) \\ &\quad + \int_0^1 d\lambda \int_P d1\; n_\lambda(1)\, w(1) \\ &\quad - \frac{i\hbar}{2}\int_0^1 d\lambda \int_P d1 \int_P d2\; \chi_\lambda(1,2) \qquad (11) \end{aligned}}$$

$$\therefore\ A = \overbrace{\langle \psi(t) | i\hbar\partial/\partial t - T | \psi(t)\rangle_{\lambda=0} - \int d1\; n(1)\, \underbrace{v_{eff}(1)}_{v(1)+w(1)}}^{A_{\lambda=0}}$$

$$- \frac{1}{2}\int_0^1 d\lambda \int_P d1 \int_P d2\, \mathcal{U}(1,2)\, n_\lambda(1)\, n_\lambda(2)$$

$$+ \int_0^1 d\lambda \int_P d1\; n_\lambda(1)\, w(1)$$

$$- \frac{i\hbar}{2}\int_0^1 d\lambda \int_P d1 \int_P d2\; \chi_\lambda(1,2)$$

$$= \langle \psi(t) | i\hbar\partial/\partial t - T | \psi(t)\rangle_{\lambda=0} - \int d1\, n(1)\, v(1) - \frac{1}{2}\int_P d1 \int_P d2\, \mathcal{U}(1,2)\, n(1)\, n(2)$$

$$+ \frac{1}{2}\int_0^1 d\lambda \int_P d1 \int_P d2\, \mathcal{U}(1,2)\, [n(1)n(2) - n_\lambda(1) n_\lambda(2)]$$

$$+ \int_0^1 d\lambda \int_P d1\; [n_\lambda(1) - n(1)]\, w(1)$$

$$- \frac{i\hbar}{2}\int_0^1 d\lambda \int_P d1 \int_P d2\; \chi_\lambda(1,2)$$

If we define the exchange-correlation part of the action through

$$\boxed{A = \langle \Psi(t) | i\hbar\partial/\partial t - T | \Psi(t) \rangle - n(\bar{1})v(\bar{1}) - \frac{1}{2}u(\bar{1},\bar{2})n(\bar{1})n(\bar{2}) + A_{xc}} \qquad (12)$$

then

$u(\bar{1},\bar{2})$

$$\boxed{\begin{aligned} A_{xc} = & -\frac{i\hbar}{2}\int_0^1 d\lambda\, \chi(\bar{1},\bar{2})_\lambda \\ & + \frac{1}{2}\int_0^1 d\lambda\, u(\bar{1},\bar{2})\,[n(1)n(2) - n_\lambda(1)n_\lambda(2)] \\ & + \int_0^1 d\lambda\, [n_\lambda(\bar{1}) - n(\bar{1})]\, w(\bar{1}) \end{aligned}} \qquad (13)$$

We temporaly neglect the terms containing $n_\lambda - n$, because the integrand equals zero for both $\lambda = 0$ and $\lambda = 1$. Then,

$$\begin{aligned} v_{xc}(1) &= \frac{\delta}{\delta n(1)}\left(-\frac{i\hbar}{2}\right)\int_0^1 d\lambda\, \chi(\bar{2},\bar{3})_\lambda \\ &= \underbrace{\frac{\delta v(4)}{\delta n(1)}}_{\chi^{-1}(4,1)}\left(-\frac{i\hbar}{2}\right)\int_0^1 d\lambda\, \underbrace{\frac{\delta \chi(\bar{2},\bar{3})_\lambda}{\delta v(4)}}_{\chi^{(3)}(\bar{2},\bar{3},\bar{4})_\lambda} \end{aligned}$$

$u(\bar{2},\bar{3})$

$$\boxed{v_{xc}(1) = -\frac{i\hbar}{2}\int_0^1 d\lambda\, \chi^{(3)}(\bar{2},\bar{3},\bar{4})_\lambda\, \chi^{-1}(\bar{4},1)} \qquad (14)$$

§. Luttinger-Ward Form

From Eq. (12),

$$A_{xc} = A - (\underbrace{\langle \psi(t) | i\hbar\partial/\partial t - T | \psi(t)\rangle}_{A_{\lambda=0} + n\underbrace{v_{eff}}_{\cancel{v} + w}} - \cancel{nv} - \frac{1}{2}unn)$$

$$= \underbrace{A - A_{\lambda=0}}_{2i(W - W_{\lambda=0}) = -2i\hbar\, tr[\ln(1-\Sigma g_0) + \Sigma g] + v_{xc}n + 2i\hbar\Xi} - nw + \frac{1}{2}unn$$

$$= -2i\hbar\, tr[\ln(1-\Sigma g_0) + \Sigma g] + 2i\hbar\Xi$$

$$+ n(\underbrace{-w + \frac{1}{2}un + v_{xc}}_{-v_{ind} - \cancel{v_{xc}} + \frac{1}{2}v_{ind} + \cancel{v_{xc}}})$$

$$\boxed{A_{xc} = -2i\hbar\, tr[\ln(1-\Sigma g_0) + \Sigma g] + 2i\hbar\Xi - \frac{1}{2}unn \rightsquigarrow ? \qquad (15)}$$

If we regard v_{eff} and w independent and take the functional derivative, then

$$A - A_{\lambda=0} =$$
$$= 2i\,(W - W_{\lambda=0})$$
$$= -2i\hbar\, \mathrm{tr}[\ln(1-\Sigma \mathcal{G}_0) + \Sigma \mathcal{G}] + \tfrac{1}{2} u n n + v_{xc} n + 2i\hbar\, \Xi$$

$$\therefore A_{xc} = (A - A_{\lambda=0}) - w n + \tfrac{1}{2} u n n$$
$$= -2i\hbar\, \mathrm{tr}[\ln(1-\Sigma \mathcal{G}_0) + \Sigma \mathcal{G}] + \underbrace{u n n + v_{xc} n - w n}_{(u n + v_{xc} - w) n = 0} + 2i\hbar\, \Xi$$

$$\boxed{\therefore \quad A_{xc} = -2i\hbar\, \mathrm{tr}[\ln(1-\Sigma \mathcal{G}_0) + \Sigma \mathcal{G}] + 2i\hbar\, \Xi \qquad (16)}$$

Matrix Representation in Keldysh Formalism

1989. 10. 5

§. Single-Particle Green's Function

$$\mathcal{G}(1,1') \equiv -(i/2)\sum_\sigma \langle T[\psi_\sigma(1)\psi_\sigma^\dagger(1')]\rangle \qquad (1)$$

$$\hat{\mathcal{G}}(1,1') = \begin{pmatrix} g_{++} & g_{+-} \\ g_{-+} & g_{--} \end{pmatrix} = \begin{pmatrix} -\frac{i}{2}\sum_\sigma \langle T_+[\psi_\sigma(1)\psi_\sigma^\dagger(1')]\rangle & \frac{i}{2}\sum_\sigma \langle \psi_\sigma^\dagger(1')\psi_\sigma(1)\rangle \\ -\frac{i}{2}\sum_\sigma \langle \psi_\sigma(1)\psi_\sigma^\dagger(1')\rangle & -\frac{i}{2}\sum_\sigma \langle T_-[\psi_\sigma(1)\psi_\sigma^\dagger(1')]\rangle \end{pmatrix} \qquad (2)$$

(Physical Representation)

$$\tilde{\mathcal{G}}(1,1') = \begin{pmatrix} 0 & g_a \\ g_r & g_c \end{pmatrix} = \begin{pmatrix} 0 & \frac{i}{2}\theta(t_1'-t_1)\sum_\sigma \langle \{\psi_\sigma(1),\psi_\sigma^\dagger(1')\}\rangle \\ -\frac{i}{2}\theta(t_1-t_1')\sum_\sigma \langle \{\psi_\sigma(1),\psi_\sigma^\dagger(1')\}\rangle & -\frac{i}{2}\sum_\sigma \langle [\psi_\sigma(1),\psi_\sigma^\dagger(1')]\rangle \end{pmatrix} \qquad (3)$$

Then,

$$\hat{\mathcal{G}} = Q^{-1}\tilde{\mathcal{G}}Q, \quad \text{or} \quad \tilde{\mathcal{G}} = Q\hat{\mathcal{G}}Q^{-1} \qquad (4)$$

where

$$Q = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \quad Q^{-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \qquad (5)$$

∵

$$Q\hat{\mathcal{G}}Q^{-1} = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}\underbrace{\begin{pmatrix} g_{++} & g_{+-} \\ g_{-+} & g_{--} \end{pmatrix}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}}_{\begin{pmatrix} g_{++}-g_{+-} & g_{++}+g_{+-} \\ g_{-+}-g_{--} & g_{-+}+g_{--} \end{pmatrix}}$$

$$= \frac{1}{2}\begin{pmatrix} g_{++}-g_{+-}-g_{-+}+g_{--} & g_{++}+g_{+-}-g_{-+}-g_{--} \\ g_{++}-g_{+-}+g_{-+}-g_{--} & g_{++}+g_{--}+g_{-+}+g_{--} \end{pmatrix}$$

① $$G_{++}+G_{--} = -\frac{i}{2}\sum_\sigma\left[\theta(t_1-t_1')\langle\psi_\sigma(1)\psi^+_\sigma(1')\rangle - \theta(t_1'-t_1)\langle\psi^+_\sigma(1')\psi_\sigma(1)\rangle\right]$$
$$-\frac{i}{2}\sum_\sigma\left[\theta(t_1'-t_1)\langle\psi_\sigma(1)\psi^+_\sigma(1')\rangle - \theta(t_1-t_1')\langle\psi^+_\sigma(1')\psi_\sigma(1)\rangle\right]$$

$$= -\frac{i}{2}\sum_\sigma\langle[\psi_\sigma(1),\psi^+_\sigma(1')]\rangle = G_c(1,1')$$

$$G_{+-}+G_{-+} = -\frac{i}{2}\sum_\sigma\langle[\psi_\sigma(1),\psi^+_\sigma(1')]\rangle = G_c(1,1')$$

② $$G_{++}-G_{+-} = -\frac{i}{2}\sum_\sigma\left[\theta(11')\langle 11'\rangle - \cancel{\theta(1'1)\langle 1'1\rangle}\right]$$
$$-\frac{i}{2}\sum_\sigma\left[\theta(11')\langle 1'1\rangle + \cancel{\theta(1'1)\langle 1'1\rangle}\right]$$
$$= -\frac{i}{2}\theta(11')\sum_\sigma\langle\{1,1'\}\rangle = G_r$$

$$G_{-+}-G_{--} = -\frac{i}{2}\sum_\sigma\left[\theta(11')\langle 11'\rangle + \cancel{\theta(1'1)\langle 11'\rangle}\right]$$
$$+\frac{i}{2}\sum_\sigma\left[\cancel{\theta(1'1)\langle 11'\rangle} - \theta(11')\langle 1'1\rangle\right]$$
$$= -\frac{i}{2}\theta(11')\sum_\sigma\langle\{1,1'\}\rangle = G_r$$

③ $$G_{++}-G_{-+} = -\frac{i}{2}\sum_\sigma\left[\cancel{\theta(11')\langle 11'\rangle} - \theta(1'1)\langle 1'1\rangle\right]$$
$$+\frac{i}{2}\sum_\sigma\left[\cancel{\theta(11')\langle 11'\rangle} + \theta(1'1)\langle 11'\rangle\right]$$
$$= \frac{i}{2}\theta(1'1)\sum_\sigma\langle\{1,1'\}\rangle = G_a$$

$$G_{+-}-G_{--} = \frac{i}{2}\sum_\sigma\left[\cancel{\theta(11')\langle 1'1\rangle} + \theta(1'1)\langle 1'1\rangle\right]$$
$$+\frac{i}{2}\sum_\sigma\left[\theta(1'1)\langle 11'\rangle - \cancel{\theta(11')\langle 1'1\rangle}\right]$$
$$= \frac{i}{2}\theta(1'1)\sum_\sigma\langle\{1,1'\}\rangle = G_a$$

① $$G_{++}+G_{--} = G_{+-}+G_{-+} = G_c \qquad \left(\overset{c}{\times}\right) \qquad (6)$$

② $$G_{++}-G_{+-} = G_{-+}-G_{--} = G_r \qquad \left(\substack{\xrightarrow{r}\\ \longrightarrow}\right) \qquad (7)$$

③ $$G_{++}-G_{-+} = G_{+-}-G_{--} = G_a \qquad \left(\downarrow\overset{a}{}\downarrow\right) \qquad (8)$$

Using these definitions,

$$Q\hat{g}Q^{-1} = \frac{1}{2}\begin{pmatrix} g_c - g_c & g_a + g_a \\ g_r + g_r & g_c + g_c \end{pmatrix} = \tilde{g} \quad //$$

§. Self-Energy

The Dyson equation is written as

$$\Gamma(1,\bar{2})\,\mathcal{G}(\bar{2},1') = \delta(1,1') \tag{9}$$

where

$$\begin{cases} \Gamma(1,2) = [i\frac{\partial}{\partial t_1} - \frac{\hbar}{2m}\nabla_1^2 - \frac{1}{\hbar}U(1,\bar{3})n(\bar{3})]\,\delta(1,2) - \frac{1}{\hbar}\Phi(1,2) - \Sigma(1,2) & (10) \\ \Sigma(1,2) = -\frac{1}{2}U(1^+,\bar{2})\,\chi^{(2)}(\bar{3},1;\bar{2}^+,\bar{2})\,\mathcal{G}^{-1}(\bar{3},1') & (11) \end{cases}$$

The matrix representation of arbitrary quantity is defined as

$$\hat{a}(1,1') = \begin{pmatrix} a_{(1,1')\in(+,+)} & a_{(+-)} \\ a_{(-+)} & a_{(--)} \end{pmatrix} \tag{12}$$

In particular,

$$\hat{\delta}(1,1') = \begin{pmatrix} \delta(1,1') & 0 \\ 0 & -\delta(1,1') \end{pmatrix} = \delta(1,1')\,\sigma_3 \tag{13}$$

where

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{14}$$

Note that,

$$\int_P dt\, f(t) = \int_{-\infty}^{\infty} dt\, f_+(t) + \int_{\infty}^{-\infty} dt\, f_-(t) = \sum_{\alpha=\pm} (-1)^{\alpha} \int_{-\infty}^{\infty} dt\, \hat{f}_{\alpha}(t) \tag{15}$$

Equation (9) may be rewritten as

$$\underbrace{\sum_{\gamma} \hat{\Gamma}_{\alpha\gamma}(1,\bar{2})(-1)^{\gamma}\hat{G}_{\gamma\beta}(\bar{2},1')}_{\sum_{\gamma\delta} \hat{\Gamma}_{\alpha\gamma}(1,\bar{2})\,\sigma_3^{\gamma\delta}\,\hat{G}_{\delta\beta}(\bar{2},1')} = \delta(1,1')\,\sigma_3^{\alpha\beta}$$

In matrix notation,

$$\hat{\Gamma}(1,\bar{2})\,\sigma_3\,\hat{G}(\bar{2},1') = \sigma_3\,\delta(1,1') \tag{16}$$

(Physical Representation)

$$\tilde{\Gamma}(1,2) \equiv Q\,\hat{\Gamma}\,Q^{-1} = \begin{pmatrix} 0^{*} & \Gamma_a \\ \Gamma_r & \Gamma_c \end{pmatrix} \tag{17}$$

then

$$\tilde{\Gamma}(1,\bar{2})\,\sigma_1\,\tilde{G}(\bar{2},1') = \sigma_1\,\delta(1,1') \tag{18}$$

where

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{19}$$

(18)

$$Q \times \text{Eq.}(16) \times Q^{-1}$$

$$\underbrace{Q\,\hat{\Gamma}(1,\bar{2})\,Q^{-1}}_{\tilde{\Gamma}(1,\bar{2})}\,Q\sigma_3 Q^{-1}\,\underbrace{Q\,\hat{g}(\bar{2},1')\,Q^{-1}}_{\tilde{g}(\bar{2},1')} = Q\sigma_3 Q^{-1}\,\delta(1,1')$$

and

$$Q\sigma_3 Q^{-1} = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 0 & 2 \\ 2 & 0 \end{pmatrix} = \sigma_1$$

*)

From Eq. (16),

$$\begin{pmatrix} \Gamma_{++}g_{++} - \Gamma_{+-}g_{-+}\;^{ⓐ} & \Gamma_{++}g_{+-} - \Gamma_{+-}g_{--}\;^{ⓑ} \\ \Gamma_{-+}g_{++} - \Gamma_{--}g_{-+}\;^{ⓒ} & \Gamma_{-+}g_{+-} - \Gamma_{--}g_{--}\;^{ⓓ} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

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$$\Gamma_{++}\underbrace{(g_{++}-g_{+-})}_{g_r} - \Gamma_{+-}\underbrace{(g_{-+}-g_{--})}_{g_r} - \Gamma_{-+}\underbrace{(g_{++}-g_{+-})}_{g_r} + \Gamma_{--}\underbrace{(g_{-+}-g_{--})}_{g_r} = 0$$

$$(\Gamma_{++} + \Gamma_{--} - \Gamma_{+-} - \Gamma_{-+})\,g_r = 0$$

$$\boxed{\therefore\ \Gamma_{++} + \Gamma_{--} = \Gamma_{+-} + \Gamma_{-+} \qquad (20)}$$

It follows from the definition of $\tilde{\Gamma}$ that $\tilde{\Gamma}_{11} = 0$. //

§. Density Response Function

$$\boxed{\chi(1,2) \equiv -\frac{i}{\hbar}\langle T[\delta\rho(1)\delta\rho(2)]\rangle \qquad (21)}$$

then

$$\boxed{\hat{\chi}(1,2) = \begin{pmatrix} \chi_{++} & \chi_{+-} \\ \chi_{-+} & \chi_{--} \end{pmatrix} = \begin{pmatrix} -\frac{i}{\hbar}\langle T_+[\delta\rho(1)\delta\rho(2)]\rangle & -\frac{i}{\hbar}\langle \delta\rho(2)\delta\rho(1)\rangle \\ -\frac{i}{\hbar}\langle \delta\rho(1)\delta\rho(2)\rangle & -\frac{i}{\hbar}\langle T_-[\delta\rho(1)\delta\rho(2)]\rangle \end{pmatrix} \qquad (22)}$$

Here,

① $\chi_{++}+\chi_{--} = -\frac{i}{\hbar}[\theta(12)\langle 12\rangle + \theta(21)\langle 12\rangle + \theta(21)\langle 12\rangle + \theta(12)\langle 21\rangle]$

$\qquad = -\frac{i}{\hbar}\langle\{1,2\}\rangle \equiv \chi_c$

then

$\chi_{+-}+\chi_{-+} = -\frac{i}{\hbar}\langle\{1,2\}\rangle = \chi_c$

② $\chi_{++}-\chi_{+-} = -\frac{i}{\hbar}[\theta(12)\langle 12\rangle + \cancel{\theta(21)\langle 21\rangle} - \theta(12)\langle 21\rangle - \cancel{\theta(21)\langle 21\rangle}]$

$\qquad = -\frac{i}{\hbar}\theta(12)\langle[1,2]\rangle \equiv \chi_r$

$\chi_{-+}-\chi_{--} = -\frac{i}{\hbar}[\theta(12)\langle 12\rangle + \cancel{\theta(21)\langle 12\rangle} - \cancel{\theta(21)\langle 12\rangle} - \theta(12)\langle 21\rangle]$

$\qquad = -\frac{i}{\hbar}\theta(12)\langle[1,2]\rangle = \chi_r$

③ $\chi_{++}-\chi_{-+} = -\frac{i}{\hbar}[\cancel{\theta(12)\langle 12\rangle} + \theta(21)\langle 21\rangle - \cancel{\theta(12)\langle 12\rangle} - \theta(21)\langle 12\rangle]$

$\qquad = \frac{i}{\hbar}\theta(21)\langle[1,2]\rangle \equiv \chi_a$

$\chi_{+-}-\chi_{--} = -\frac{i}{\hbar}[\cancel{\theta(12)\langle 21\rangle} + \theta(21)\langle 21\rangle - \cancel{\theta(12)\langle 21\rangle} - \theta(21)\langle 12\rangle]$

$\qquad = \frac{i}{\hbar}\theta(21)\langle[1,2]\rangle = \chi_a$

$$\chi_r(1,2) \equiv -\frac{i}{\hbar}\Theta(t_1-t_2)\langle[\delta\rho(1),\delta\rho(2)]\rangle \tag{23}$$

$$\chi_a(1,2) \equiv \frac{i}{\hbar}\Theta(t_2-t_1)\langle[\delta\rho(1),\delta\rho(2)]\rangle \tag{24}$$

$$\chi_c(1,2) \equiv -\frac{i}{\hbar}\langle\{\delta\rho(1),\delta\rho(2)\}\rangle \tag{25}$$

① $$\chi_{++} + \chi_{--} = \chi_{+-} + \chi_{-+} = \chi_c \tag{26}$$

② $$\chi_{++} - \chi_{+-} = \chi_{-+} - \chi_{--} = \chi_r \tag{27}$$

③ $$\chi_{++} - \chi_{-+} = \chi_{+-} - \chi_{--} = \chi_a \tag{28}$$

These equations have the same structure as that of Eqs. (6)–(8), so that

$$\tilde{\chi} = \begin{pmatrix} 0 & \chi_a \\ \chi_r & \chi_c \end{pmatrix} = Q\,\hat{\chi}\,Q^{-1} \tag{29}$$

§. Physical Response

Physical system is obtained by setting

$$\hat{\phi}(1,1') = \begin{pmatrix} \phi(1)\delta(11') & 0 \\ 0 & \phi(1)\delta(11') \end{pmatrix} = \delta(11')\mathbb{1} \tag{30}$$

Then,

$$\delta f = \int_p d1 \frac{\delta f}{\delta\phi(1)} \delta\phi(1)$$

$$= \int_{-\infty}^{\infty} d1 \left(\frac{\delta f}{\delta\phi_+(1)} - \frac{\delta f}{\delta\phi_-(1)} \right)_{\phi_+\to\phi_-} \delta\phi(1)$$

$$\boxed{\therefore \frac{\delta f}{\delta\phi(1)} = \left[\frac{\delta}{\delta\phi_+(1)} - \frac{\delta}{\delta\phi_-(1)} \right] f \Big|_{\phi_+=\phi_-} = \sum_\sigma \sigma \frac{\delta}{\delta\phi_\sigma(1)} f \Big|_{\phi_\sigma=\phi}} \tag{31}$$

(Linear Response)

$$\frac{\delta n_\pm(1)}{\delta\phi(2)} = \frac{\delta n_\pm(1)}{\delta\phi_+(2)} - \frac{\delta n_\pm(1)}{\delta\phi_-(2)}$$

$$= \chi_{\pm+}(1,2) - \chi_{\pm-}(1,2) = \chi_r(1,2) \tag{32}$$

(Quadratic Response)

$$\frac{\delta^2 n_\pm(1)}{\delta\phi(3)\delta\phi(2)} = \left[\frac{\delta}{\delta\phi_+(3)} - \frac{\delta}{\delta\phi_-(3)} \right] \left[\chi_{\pm+}(1,2) - \chi_{\pm-}(1,2) \right]$$

$$= \chi^{(3)}_{\pm++}(1,2,3) - \chi^{(3)}_{\pm+-}(1,2,3)$$
$$- \chi^{(3)}_{\pm+-}(1,2,3) - \chi^{(3)}_{\pm--}(1,2,3)$$

$$\boxed{\therefore \frac{\delta^2 n_\sigma(1)}{\delta\phi(3)\delta\phi(2)} = \sum_{\tau\upsilon=\pm} \tau\upsilon\, \chi^{(3)}_{\sigma\tau\upsilon}(1,2,3)} \tag{34}$$

8. Physical Expressions

$$\hat{g} = \frac{1}{2} Q^{-1} \tilde{g} Q$$

$$= \frac{1}{2} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} 0 & g_a \\ g_r & g_c \end{pmatrix} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$$

$$= \frac{1}{2} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} a & a \\ r+c & -r+c \end{pmatrix}$$

$$= \frac{1}{2} \begin{pmatrix} a+r+c & a-r+c \\ -a+r+c & -a-r+c \end{pmatrix}$$

$$\boxed{\hat{g} = \begin{pmatrix} g_{++} & g_{+-} \\ g_{-+} & g_{--} \end{pmatrix} = \frac{1}{2} \left\{ g_r \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix} + g_a \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} + g_c \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \right\}} \qquad (35)$$

The same for χ.

Physical Representation of XC Potentials

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§. Linear Response

First, note that

$$\frac{\delta f}{\delta \phi(1)} = \sum_{\sigma=\pm} \sigma \frac{\delta}{\delta \phi_\sigma(1)} f \Big|_{\phi_\sigma \to \phi} \qquad (1)$$

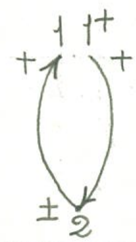
Since $n(1) = -2i\mathcal{G}_{++}(1,1^+) = -2i\mathcal{G}_{--}(1,1^-) = -2i\mathcal{G}_{+-}(1,1)$, we first examine these three choices in the lowest-order approximations.

① $-\frac{2i}{\hbar}\left[\mathcal{G}_{++}(1,2)\mathcal{G}_{++}(2,1) - \mathcal{G}_{+-}(1,2)\mathcal{G}_{-+}(2,1)\right]$

$$= -\frac{\cancel{2}i}{\hbar}\times\frac{1}{\cancel{4}\,2}\left[\underbrace{(r+a+c)(r+a+c) - (-r+a+c)(r-a+c)}\right]$$

$$\begin{array}{rl} & rr + \cancel{ra} + rc + \cancel{ar} + aa + \cancel{ac} + \cancel{cr} + ca + \cancel{cc} \\ -) & -rr + \cancel{ra} - rc + \cancel{ar} - aa + \cancel{ac} + \cancel{cr} - ca + \cancel{cc} \\ \hline & \cancel{2}(rr + rc + aa + ca) \end{array}$$

$$\boxed{\begin{aligned} &-2i\hbar^{-1}\sum_\sigma \sigma \mathcal{G}_{+\sigma}(1,2)\mathcal{G}_{\sigma+}(2,1) \\ &= -i\hbar^{-1}(\mathcal{G}_r\mathcal{G}_c + \mathcal{G}_c\mathcal{G}_a + \mathcal{G}_r\mathcal{G}_r + \mathcal{G}_a\mathcal{G}_a) \qquad (2a) \\ &= -i\hbar^{-1}(\mathcal{G}_r\mathcal{G}_c + \mathcal{G}_c\mathcal{G}_a) \qquad (2b) \end{aligned}}$$



($\because$ $\mathcal{G}_r(1,2)\mathcal{G}_r(2,1) \sim \theta(t_1-t_2)\theta(t_2-t_1) = 0$.)

② $-\frac{2i}{\hbar}\left[\mathcal{G}_{-+}(12)\mathcal{G}_{+-}(21) - \mathcal{G}_{--}(12)\mathcal{G}_{--}(21)\right]$

$$= -\frac{i}{2\hbar}\left[\underbrace{(r-a+c)(-r+a+c) - (-r-a+c)(-r-a+c)}\right]$$

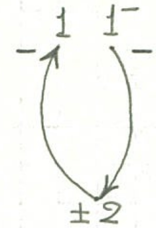
$$\begin{array}{rl} & -rr + \cancel{ra} + rc + \cancel{ar} - aa - \cancel{ac} - \cancel{cr} + ca + \cancel{cc} \\ -) & rr + \cancel{ra} - rc + \cancel{ar} + aa - \cancel{ac} - \cancel{cr} - ca + \cancel{cc} \\ \hline & 2(-rr + rc - aa + ca) \end{array}$$

$$= -\frac{i}{\hbar}(rc + ca - rr - aa)$$

$$-2i\hbar^{-1}\sum_{\sigma}\sigma\, \mathcal{G}_{-\sigma}(1,2)\mathcal{G}_{\sigma-}(2,1)$$

$$= -i\hbar^{-1}(\mathcal{G}_r\mathcal{G}_c + \mathcal{G}_c\mathcal{G}_a - \mathcal{G}_r\mathcal{G}_r - \mathcal{G}_a\mathcal{G}_a) \tag{3a}$$

$$= -i\hbar^{-1}(\mathcal{G}_r\mathcal{G}_c + \mathcal{G}_c\mathcal{G}_a) \tag{3b}$$



③ $-\frac{2i}{\hbar}[\mathcal{G}_{++}(12)\mathcal{G}_{+-}(21) - \mathcal{G}_{+-}(12)\mathcal{G}_{--}(21)]$

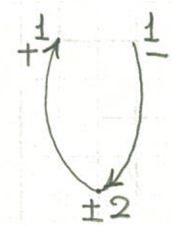
$$= -\frac{i}{2\hbar}[\underbrace{(r+a+c)(-r+a+c)}-(-r+a+c)(-r-a+c)]$$

$$\begin{array}{rl} & -rr + r\cancel{a} + rc - a\cancel{r} + aa + a\cancel{c} - c\cancel{r} + ca + c\cancel{c} \\ -) & rr + \cancel{r}a - rc - \cancel{a}r - aa + \cancel{a}c - \cancel{c}r - ca + \cancel{c}c \\ \hline & 2(-rr + rc + aa + ca) \end{array}$$

$$-2i\hbar^{-1}\sum_{\sigma}\sigma\, \mathcal{G}_{+\sigma}(1,2)\mathcal{G}_{\sigma-}(2,1)$$

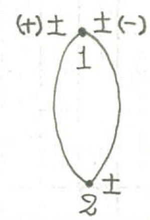
$$= -i\hbar^{-1}(\mathcal{G}_r\mathcal{G}_c + \mathcal{G}_c\mathcal{G}_a - \mathcal{G}_r\mathcal{G}_r + \mathcal{G}_a\mathcal{G}_a) \tag{4a}$$

$$= -i\hbar^{-1}(\mathcal{G}_r\mathcal{G}_c + \mathcal{G}_c\mathcal{G}_a) \tag{4b}$$



$$\therefore \chi_{\sigma r}(1,2) = -2i\hbar^{-1}\sum_{\tau}\tau\, \mathcal{G}_{\sigma\tau}(1,2)\mathcal{G}_{\tau\sigma'}(2,1) \quad (\sigma,\sigma') = (\pm,\pm) \text{ or } (+,-) \tag{5a}$$

$$= -i\hbar^{-1}(\mathcal{G}_r\mathcal{G}_c + \mathcal{G}_c\mathcal{G}_a) \tag{5b}$$



This is consistent with a more general formula,

$$\frac{\delta n_\sigma(1)}{\delta\phi(2)} = \sum_{\tau}\tau\frac{\delta n_\sigma}{\delta\phi_\tau}\Big|_{\phi_\tau\to\phi} = \chi_{\sigma+} - \chi_{\sigma-} = \chi_r(1,2) \tag{6}$$

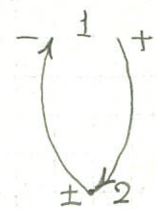
However, the other choice $(\sigma,\sigma') = (-,+)$ does not apply to this case.

④ $$-\frac{2i}{\hbar}\left[\mathcal{G}_{-+}(12)\mathcal{G}_{++}(21) - \mathcal{G}_{--}(12)\mathcal{G}_{-+}(21)\right]$$

$$= -\frac{i}{2\hbar}\Big[\underbrace{(r-a+c)(r+a+c) - (-r-a+c)(r-a+c)}\Big]$$

$$\begin{array}{rl} & rr + \cancel{ra} + rc - \cancel{ar} - aa - \cancel{ac} + \cancel{cr} + ca + \cancel{cc} \\ -) & -rr + \cancel{ra} - rc - \cancel{ar} + aa - \cancel{ac} + \cancel{cr} - ca + \cancel{cc} \\ \hline & 2(rr + rc - aa + ca) \end{array}$$

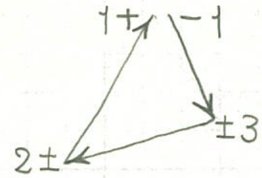
$$\boxed{\begin{aligned} & -2i\hbar^{-1}\sum_{\sigma}\sigma\,\mathcal{G}_{-\sigma}(1,2)\,\mathcal{G}_{\sigma+}(2,1) \\ &= -i\hbar^{-1}(\mathcal{G}_r\mathcal{G}_c + \mathcal{G}_c\mathcal{G}_a + \mathcal{G}_r\mathcal{G}_r - \mathcal{G}_a\mathcal{G}_a) \qquad (7a) \\ &= -i\hbar^{-1}(\mathcal{G}_r\mathcal{G}_c + \mathcal{G}_c\mathcal{G}_a) = \chi_r(1,2) \qquad (7b) \end{aligned}}$$



Nevertheless, χ_r is also reproduced in this case.

§. Nonlinear Response

$$\chi_0^{(3)}(1,2,3) = -\frac{2i}{\hbar^2}\sum_{\tau\upsilon}\tau\upsilon\left[g_{+\tau}(1,2)\,g_{\tau\upsilon}(2,3)\,g_{\upsilon-}(3,1) + (2\longleftrightarrow 3)\right] \quad (8)$$



$$\mathcal{C} = \sum_{\tau\upsilon}\tau\upsilon\left[g_{+\tau}(12)\,g_{\tau\upsilon}(23)\,g_{\upsilon-}(31)\right]$$

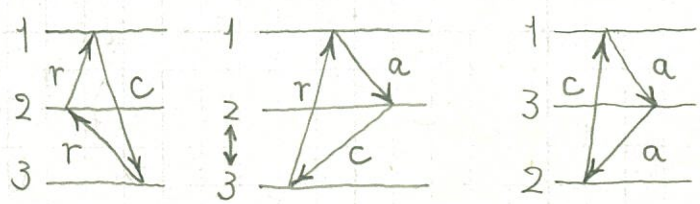
$$= g_{++}\underbrace{(g_{++}g_{+-} - g_{+-}g_{--})}_{\frac{1}{2}(rc+ca-rr+aa)} - g_{+-}\underbrace{(g_{-+}g_{+-} - g_{--}g_{--})}_{\frac{1}{2}(rc+ca-rr-aa)}$$

$$= \frac{1}{2}\underbrace{(g_{++}-g_{+-})}_{r}(rc+ca-rr) + \frac{1}{2}\underbrace{(g_{++}+g_{+-})}_{\frac{1}{2}(\cancel{r}+a+c-\cancel{r}+a+c) = a+c}aa$$

$$= \frac{1}{2}(rrc + rca - \cancel{rrr} + \cancel{aaa} + caa)$$

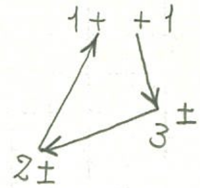
$$\hookrightarrow \theta(t_1-t_2)\,\theta(t_2-t_3)\,\theta(t_3-t_1) = 0$$

$$\chi_0^{(3)}(1,2,3) = -\frac{i}{\hbar^2}\Big[g_r(12)\,g_r(23)\,g_c(31) + g_r(12)\,g_c(23)\,g_a(31) + g_c(12)\,g_a(23)\,g_a(31) + (2\leftrightarrow 3)\Big] \quad (9)$$



※ We may use other end-point signs $(\pm,\pm)$.

$$\alpha' = \sum_{\tau\upsilon} \tau\upsilon \left[g_{+\tau}(12)\, g_{\tau\upsilon}(23)\, g_{\upsilon+}(31) \right]$$



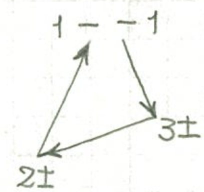
$$= g_{++}(\underbrace{g_{++}g_{++} - g_{+-}g_{-+}}_{\frac{1}{2}(rc+ca+rr+aa)}) - g_{+-}(\underbrace{g_{-+}g_{++} - g_{--}g_{-+}}_{\frac{1}{2}(rc+ca+rr-aa)})$$

$$= \frac{1}{2}(\underbrace{g_{++} - g_{+-}}_{r})(rc+ca+rr) + \frac{1}{2}(\underbrace{g_{++} + g_{+-}}_{\frac{1}{2}(\cancel{r}+a+c-\cancel{r}+a+c) = a+c})\, aa$$

$$= \frac{1}{2}(rrc + rca + \cancel{rrr} + \cancel{aaa} + caa)$$

$$= \alpha$$

$$\alpha'' = \sum_{\tau\upsilon} \tau\upsilon \left[g_{-\tau}(12)\, g_{\tau\upsilon}(23)\, g_{\upsilon-}(31) \right]$$



$$= g_{-+}(\underbrace{g_{++}g_{+-} - g_{+-}g_{--}}_{\frac{1}{2}(rc+ca-rr+aa)}) - g_{--}(\underbrace{g_{-+}g_{+-} - g_{--}g_{--}}_{\frac{1}{2}(rc+ca-rr-aa)})$$

$$= \frac{1}{2}(\underbrace{g_{-+} - g_{--}}_{r})(rc+ca-rr) + \frac{1}{2}(\underbrace{g_{-+} + g_{--}}_{\frac{1}{2}(\cancel{r}-a+c-\cancel{r}-a+c) = -a+c})\, aa$$

$$= \frac{1}{2}(rrc + rca - \cancel{rrr} - \cancel{aaa} + caa)$$

$$= \alpha$$

//

§. Physical Sham Equation

Now it is obvious that

① $\chi_{eff}^{-1}(1,\bar{2})f(\bar{2})\Big|_{f_+=f_-} = \chi_{eff;r}^{-1}(1,\bar{2})f(\bar{2})$ (10)

② $\mathcal{G}_0(2,\bar{3})\Sigma_{xc}(\bar{3},\bar{4})\mathcal{G}(\bar{4},2)$ for any end-point signs

$$= \frac{1}{2}[\mathcal{G}_0^r\Sigma_{xc}^r\mathcal{G}^c + \mathcal{G}_0^r\Sigma_{xc}^c\mathcal{G}^a + \mathcal{G}_0^c\Sigma_{xc}^a\mathcal{G}^a] \qquad (11)$$

Using these relations,

$$v_{xc}(1) = -2i\,\pi^{-1}(1,\bar{2})\mathcal{G}_0(\bar{2},\bar{3})\Sigma_{xc}(\bar{3},\bar{4})\mathcal{G}(\bar{4},\bar{2}) \qquad (12a)$$

$$= -2i\pi_r^{-1}[\mathcal{G}_0^r\Sigma_{xc}^r\mathcal{G}^c + \mathcal{G}_0^r\Sigma_{xc}^c\mathcal{G}^a + \mathcal{G}_0^c\Sigma_{xc}^a\mathcal{G}^a] \qquad (12b)$$

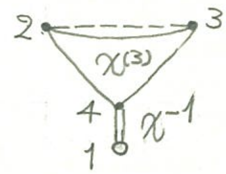
where

$$\pi(1,2) = -2i\hbar^{-1}\mathcal{G}_0(1,2)\mathcal{G}(2,1) \qquad (13a)$$

$$\pi_r(1,2) = -2i\hbar^{-1}(\mathcal{G}_0^r\mathcal{G}^c + \mathcal{G}_0^c\mathcal{G}^a) \qquad (13b)$$

§ Physical Correlation Representation

$$v_{xc}(1) = -i\hbar 2^{-1}\int_0^1 d\lambda\, u(\bar{r}_2-\bar{r}_3)\, \chi^{(3)}(\bar{r}_2,\bar{t}_2;\bar{r}_3,\bar{t}_2;\bar{4})_\lambda\, \chi^{-1}(\bar{4},1) \tag{14}$$



Here,

$$\begin{aligned}
& f(\bar{3},\bar{4})\, g(\bar{4},1) \\
&= \sum_{\tau\upsilon} \tau\upsilon\, f_{\tau\upsilon}(\bar{3},\bar{4})\, g_{\upsilon+}(\bar{4},1) \\
&= \underbrace{f_{++}g_{++} - f_{+-}g_{-+}}_{\frac{1}{2}(rc+ca+rr+aa)} - \underbrace{f_{-+}g_{++} + f_{--}g_{-+}}_{\frac{1}{2}(rc+ca+rr-aa)} \\
&= \tfrac{1}{2}(\cancel{rc}+\cancel{ca}+\cancel{rr}+aa-\cancel{rc}-\cancel{ca}-\cancel{rr}+aa) = \underline{aa}
\end{aligned}$$

$$\boxed{\begin{aligned}
v_{xc}(1) &= -\frac{i\hbar}{2}\int_0^1 d\lambda\, u(\bar{2},\bar{3})\, \chi^{(3)}(\bar{2},\bar{3},\bar{4})_\lambda\, \chi^{-1}(\bar{4},1) && (15a) \\
&= -\frac{i\hbar}{2}\int_0^1 d\lambda\, u(\bar{r}_2-\bar{r}_3)\, \chi_a^{(3)}(\bar{r}_2,\bar{t}_2;\bar{r}_3,\bar{t}_2;\bar{4})_\lambda\, \chi_a^{-1}(\bar{4},1) && (15b)
\end{aligned}}$$

§. Kohn-Sham Scheme

$$g_{+-}(11') = \frac{i}{2}\sum_{\sigma} \langle 0|\underbrace{\psi^{+}_{\sigma}(1')}_{\sum_j \phi^*_{j\sigma}(1')\,a^{+}_{j\sigma}}\underbrace{\psi_{\sigma}(1)}_{\sum_i \phi_{i\sigma}(1)\,a_{i\sigma}}|0\rangle$$

$$= \frac{i}{2}\sum_{ij\sigma} \phi^*_{j\sigma}(1')\phi_{i\sigma}(1) \quad \langle 0|a^{+}_{j\sigma}a_{i\sigma}|0\rangle$$

Now, assume

$$|0\rangle = \prod_{j\lambda}^{N} a^{+}_{j\lambda}\,|v\rangle \tag{16}$$

Then, only the terms $i=j$ survives and

$$g_{+-}(11') = \frac{i}{2}\sum_{i\sigma} \phi^*_{i\sigma}(1')\phi_{i\sigma}(1) \quad \underbrace{\langle 0|\underbrace{a^{+}_{i\sigma}a_{i\sigma}|0\rangle}_{|0\rangle}}_{=1 \text{ if } i\sigma \text{ is filled.}}$$

In the same way

$$g_{-+}(11') = -\frac{i}{2}\sum_{i\sigma} \phi_{i\sigma}(1)\phi^*_{i\sigma}(1') \quad \underbrace{\langle 0|a_{i\sigma}a^{+}_{i\sigma}|0\rangle}_{=1 \text{ if } i\sigma \text{ is unfilled.}}$$

$$\boxed{\begin{aligned} g_{+-}(1,1') &= \frac{i}{2}\sum_{i\sigma} \phi_{i\sigma}(1)\phi^*_{i\sigma}(1')\,f_{i\sigma} && (17) \\ g_{-+}(1,1') &= -\frac{i}{2}\sum_{i\sigma} \phi_{i\sigma}(1)\phi^*_{i\sigma}(1')\,(1-f_{i\sigma}) && (18) \end{aligned}}$$

① $$\mathcal{G}_r(1,1') = \Theta(t_1-t_1') \sum_{i\sigma} \phi_{i\sigma}(1)\phi^*_{i\sigma}(1')\left(-\frac{i}{2}\right)(\cancel{f_{i\sigma}} + 1 - \cancel{f_{i\sigma}})$$

② $$\mathcal{G}_a(1,1') = \frac{i}{2}\Theta(t_1'-t_1) \sum_{i\sigma} \phi_{i\sigma}(1)\phi^*_{i\sigma}(1')\ (\cancel{f_{i\sigma}} + 1 - \cancel{f_{i\sigma}})$$

③ $$\mathcal{G}_c(1,1') = -\frac{i}{2}\sum_{i\sigma} \phi_{i\sigma}(1)\phi^*_{i\sigma}(1')\ (1 - f_{i\sigma} - f_{i\sigma})$$

$$\boxed{\begin{cases} \mathcal{G}_r(1,1') = -\frac{i}{2}\Theta(t_1-t_1')\sum_{i\sigma}\phi_{i\sigma}(1)\phi^*_{i\sigma}(1') & (19) \\ \mathcal{G}_a(1,1') = \frac{i}{2}\Theta(t_1'-t_1)\sum_{i\sigma}\phi_{i\sigma}(1)\phi^*_{i\sigma}(1') & (20) \\ \mathcal{G}_c(1,1') = -\frac{i}{2}\sum_{i\sigma}\phi_{i\sigma}(1)\phi^*_{i\sigma}(1')(1-2f_{i\sigma}) & (21) \end{cases}}$$

$$\chi_{0r}(1,2) = -\frac{2i}{\hbar}\left[\underbrace{\mathcal{G}_r(12)\mathcal{G}_c(21)} + \underbrace{\mathcal{G}_c(12)\mathcal{G}_a(21)}\right]$$

$$-\frac{1}{4}\Theta(t_1-t_2)\sum_{\substack{i\sigma\\ j\lambda}}\phi_{i\sigma}(1)\phi^*_{i\sigma}(2)\phi_{j\lambda}(2)\phi^*_{j\lambda}(1)\ (\cancel{1} - 2f_{j\lambda})$$

$$+\frac{1}{4}\Theta(t_1-t_2)\sum_{\substack{i\sigma\\ j\lambda}}\phi_{i\sigma}(1)\phi^*_{i\sigma}(2)(\cancel{1}-2f_{i\sigma})\ \phi_{j\lambda}(2)\phi^*_{j\lambda}(1)$$

$$= -\frac{\cancel{2}i}{\hbar}\cdot\frac{1}{\cancel{4}}\cancel{2}\,\Theta(t_1-t_2)\sum_{\substack{ij\\ \sigma\lambda}}\phi_{i\sigma}(1)\phi^*_{i\sigma}(2)\phi_{j\lambda}(2)\phi^*_{j\lambda}(1)\,(f_{i\sigma}-f_{j\lambda})$$

$$\boxed{\chi_{0r}(1,2) = -i\hbar^{-1}\Theta(t_1-t_2)\sum_{\substack{ij\\ \sigma\lambda}}\phi_{i\sigma}(1)\phi^*_{i\sigma}(2)\phi_{j\lambda}(2)\phi^*_{j\lambda}(1)\,(f_{i\sigma}-f_{j\lambda}) \qquad (22)}$$

The XC Potential : Self-Energy Formula

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§. Definitions

(System)

$$H(t) = T + U + V(t) \tag{1}$$

$$\begin{cases} T = \sum_\sigma \int d^3r\, \psi_\sigma^\dagger(r)\,(-\hbar^2\nabla^2/2m)\,\psi_\sigma(r) & (2) \\ U = \frac{1}{2}\sum_{\sigma\sigma'} \int d^3r \int d^3r'\, \psi_\sigma^\dagger(r)\,\psi_{\sigma'}^\dagger(r')\,u(r-r')\,\psi_{\sigma'}(r')\,\psi_\sigma(r) & (3) \\ V(t) = \int d^3r\, \rho(r)\, v(r,t) & (4) \end{cases}$$

where $u(r) = e^2/r$, and $\rho(r) = \sum_\sigma \psi_\sigma^\dagger(r)\psi_\sigma(r)$.

(KS-based Perturbation)

$$H(t) = [\,T + V_{eff}(t)\,] + [\,U + V(t) - V_{eff}(t)\,] \tag{5a}$$

$$= \quad H_0(t) \quad + \quad H_1(t) \tag{5b}$$

Here,

$$V_{eff}(t) = \int d^3r\, \rho(r)\, \underbrace{[\, \underbrace{v(r,t) + \overbrace{\int d^3r'\, u(r-r')\, n(r',t)}^{v_{ind}(r,t)}}_{v_H(r,t)} + v_{xc}(r,t)\,]}_{v_{eff}(r,t)} \tag{6}$$

$$H_1(t) = U - \int d^3r\, \rho(r)\, [\, \underbrace{v_{ind}(r,t) + v_{xc}(r,t)}_{w(r,t)}\,] \tag{7}$$

where

$$v_{xc}(r,t) = \delta A_{xc} / \delta n(r,t) \tag{8}$$

(Generating Functional)

$$S = T_P \exp\Big[-\frac{i}{\hbar}\sum_\sigma \int_P d1 \int_P d1'\, \psi_{H\sigma}^\dagger(1)\, \phi(1,1')\, \psi_{H\sigma}(1')\,\Big] \tag{9}$$

where

$$\psi_{H\sigma}^{(\dagger)}(1) = \mathcal{U}_-(-t_0,t_1)\, \psi_\sigma^{(\dagger)}(r_1,t_1)\, \mathcal{U}_+(t_1,-t_0) \tag{10}$$

$$Z = \mathrm{tr}\,(S\hat{\rho}) \tag{11}$$

$$W = -(\hbar/2)\ln Z \tag{12}$$

Then,

$$\frac{\delta W}{\delta\phi(1',1)} = \mathcal{G}(1,1') \tag{13}$$

where the single-particle Green's function is defined as

$$\mathcal{G}(1,1') = -\frac{i}{2}\sum_{\sigma}\langle T_p[\psi_\sigma(1)\psi_\sigma^{\dagger}(1')]\rangle \tag{14}$$

and the average is defined by

$$\langle\theta(t)\rangle = Z^{-1}\mathrm{tr}\,\{T_p[\theta_H(t)S]\hat{\rho}\} \tag{15}$$

(Vertex Functional)

$$\Gamma[\mathcal{G}] = W[\Phi] - \int_p d1\int_p d1'\,\mathcal{G}(1,1')\Phi(1',1) \tag{16a}$$

$$= W - \mathrm{tr}\,(\mathcal{G}\Phi) \tag{16b}$$

Then,

$$\frac{\delta\Gamma}{\delta\mathcal{G}(1,1')} = -\Phi(1',1) \tag{17}$$

§. Dyson's Equation

Using the equation of motion for the GF,

$$\mathcal{G}^{-1}(1,1') = \mathcal{G}_0^{-1}(1,1') - \hbar^{-1}\Phi(1,1') - \Sigma(1,1') \tag{18}$$

where

$$\mathcal{G}_0^{-1}(1,1') = [i\,\partial/\partial t_1 + \hbar\nabla_1^2/2m - \hbar^{-1}\underbrace{v_{\mathrm{eff}}(1)}_{\text{external parameter}}]\,\delta_p(1,1') \tag{19}$$

$$\Sigma(1,1') = -2^{-1}U(1^+;\bar{2})\chi^{(2)}(\bar{3},1;\bar{2}^+,\bar{2})G^{-1}(\bar{3},1') - \hbar^{-1}[\overbrace{w(1)}^{\text{ext. par.}} - \overbrace{v_{ind}(1)}^{\text{dynamic var.}}]\delta_p(1,1') \tag{20}$$

$$= \Sigma_{xc}(1,1') - \hbar^{-1}v_{xc}(1)\,\delta_p(1,1') \tag{21}$$

$$\chi^{(\nu)}(1,1';\ldots;\nu,\nu') = \frac{\delta^{\nu-1}}{\delta\phi(\nu,\nu')\cdots\delta\phi(2,2')}\sum_\sigma\langle T[\psi_\sigma(1)\psi_\sigma^\dagger(1')]\rangle \tag{22}$$

※ Note that in Eq. (20), $w(1)$ is an external parameter contained in the original Hamiltonian (see Eq. (7)); on the other hand $v_{ind}(1) = U(1,\bar{2})n(\bar{2})$ derives from commutation operations, thus is a dynamic variable coupled to $\phi(1,1')$.

Comparing Eq. (17) with Eq. (18),

$$\frac{\delta\Gamma}{\delta G(1,1')} = \hbar\,[G^{-1}(1',1) - G_0^{-1}(1',1) + \Sigma(1',1)] \tag{23}$$

$$\therefore \delta\Gamma = \hbar[\underbrace{G^{-1}(\bar{1}',\bar{1})\delta G(\bar{1},\bar{1}')}_{\delta \ln G(\bar{1}',\bar{1}')} - G_0^{-1}(\bar{1}',\bar{1})\delta G(\bar{1},\bar{1}') + \underbrace{\Sigma(\bar{1}',\bar{1})\delta G(\bar{1},\bar{1}')}_{\delta\Xi}]$$

$$= \delta\,\hbar\,\mathrm{tr}[\ln G - G_0^{-1}G] + \hbar\,\Xi$$

$$\therefore \Gamma = \hbar\,\mathrm{tr}[\ln G - G_0^{-1}G] + \hbar\,\Xi \tag{24}$$

where

$$\delta\,\mathrm{tr}\ln G = G^{-1}(\bar{1}\bar{1}')\,\delta G(\bar{1}'\bar{1}) \tag{25}$$

$$\delta\Xi/\delta G(1',1) = \Sigma(1,1') \tag{26}$$

§. Generator as a Functional of $\mathcal{G}$

From Eqs. (16) and (24),

$$W = \Gamma + tr(\mathcal{G}\Phi)$$

$$= \hbar\, tr[\ln\mathcal{G} - \underbrace{(\mathcal{G}_0^{-1} - \hbar^{-1}\Phi)}_{\mathcal{G}^{-1}+\Sigma}\mathcal{G}] + \hbar\Xi$$

constant of integration, omitted!

$$\therefore W = \hbar\, tr[\ln\mathcal{G} - \Sigma\mathcal{G} - \cancel{1}] + \hbar\Xi \tag{27}$$

We here introduce a dimensionless coupling constant λ such that

$$H(t) = H_0(t) + \lambda H_1(t) \tag{28}$$

Then, for the system $\lambda = 0$,

$$W_{\lambda=0} = \hbar\, tr(\ln\mathcal{G}_0) \tag{29}$$

Subtracting Eq. (29) from Eq. (27),

$$W - W_{\lambda=0} = \hbar\, tr[\ln(\mathcal{G}/\mathcal{G}_0) - \Sigma\mathcal{G}] + \hbar\Xi$$

Consider a system $\Phi(1,1') \to 0$, then $\mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \Sigma$ from Eq. (18), so that

$$\boxed{W - W_{\lambda=0} = \hbar\, tr[\ln(\mathcal{G}/\mathcal{G}_0) - \mathcal{G}_0^{-1}\mathcal{G} + 1] + \hbar\Xi} \tag{30}$$

Eq. (5-203) in Nozières

From Eq. (20),

$$\hbar\,\mathrm{tr}(\Sigma\,\delta\mathcal{G}) = \hbar\,\mathrm{tr}(\Sigma_{xc}\delta\mathcal{G}) - w(\bar{1})\,\delta\underbrace{\mathcal{G}(\bar{1},\bar{1}^{+})}_{-\frac{i}{2}\sum_{\sigma}\langle T[\psi_{\sigma}(1)\psi_{\sigma}^{+}(1^{+})\rangle = \frac{i}{2}n(1)} + u(\bar{1},\bar{2})\,n(\bar{2})\,\delta\mathcal{G}(\bar{1},\bar{1}^{+})$$

$$= \hbar\,\mathrm{tr}(\Sigma_{xc}\delta\mathcal{G}) - \frac{i}{2}w(\bar{1})\,\delta n(\bar{1}) + \frac{i}{2}u(\bar{1},\bar{2})\,n(\bar{2})\,\delta n(\bar{1})$$

$$= \delta\left\{\hbar\,\mathrm{tr}(\Sigma_{xc}\delta\mathcal{G}) - \frac{i}{2}w(\bar{1})n(\bar{1}) + \frac{i}{4}u(\bar{1},\bar{2})\,n(\bar{1})\,n(\bar{2})\right\}$$

Then, Eq. (30) can be rewritten as

$$W - W_{\lambda=0} = \hbar\,\mathrm{tr}[\ln(\mathcal{G}/\mathcal{G}_0) - \mathcal{G}_0^{-1}\mathcal{G} + 1] - \frac{i}{2}w(\bar{1})n(\bar{1}) + \frac{i}{4}u(\bar{1},\bar{2})\,n(\bar{1})\,n(\bar{2}) + \Xi_{xc} \qquad (31)$$

where

$$\delta\Xi_{xc}/\delta\mathcal{G}(1',1) = \Sigma_{xc}(1,1')$$

§. Action Integral

$$A = \int_{-t_0}^{t_0} dt \, \langle \psi(t) | i\hbar \partial/\partial t - H(t) | \psi(t) \rangle \tag{32}$$

We now extend the action integral to the closed-time path,

$$\boxed{A = \int_P dt \, \langle \psi(t) | i\hbar \partial/\partial t - H(t) | \psi(t) \rangle} \tag{33}$$

We introduce the dimensionless coupling constant λ, Eq. (28), and differentiate Eq. (33) with respect to λ,

$$\begin{aligned} \frac{dA}{d\lambda} = \int_P dt \Big\{ \frac{d}{d\lambda} \langle \psi(t)| \Big\} \overbrace{[i\hbar \partial/\partial t - H(t)] |\psi(t)\rangle}^{\to 0} &- \langle \psi(t) | H_1(t) | \psi(t) \rangle \\ &\underline{- \langle \psi(t) | [i\hbar \partial/\partial t - H(t)] \frac{d}{d\lambda} | \psi(t) \rangle} \\ &+ \underbrace{\Big\{ i\hbar \frac{\partial}{\partial t} \langle \psi(t) | + \langle \psi(t) | H(t) \Big\}}_{\to 0} \frac{d}{d\lambda} | \psi(t) \rangle \\ = - \int_P dt \, \langle \psi(t) | H_1(t) | \psi(t) \rangle_\lambda \end{aligned}$$

$$\boxed{\therefore \; A - A_{\lambda=0} = - \int_P dt \, \langle \psi(t) | H_1(t) | \psi(t) \rangle_\lambda} \tag{34}$$

(Comparison with W)

If we temporaly assume $\phi(1,1') = \phi(1) \delta_P(1,1')$, then

$$Z = tr\{ T_P \exp[-\frac{i}{\hbar} \int_P dt \, \Phi_H(t)] \, \hat{\rho} \} = tr(S\hat{\rho}) \tag{35a}$$

$$= tr\{ T_P \exp[-\frac{i}{\hbar} \int_P dt \, (H_{1H_0}(t) + \Phi_{H_0}(t))] \hat{\rho} \} = tr(S_0 \hat{\rho}) \tag{35b}$$

where

$$\Phi(t) = \int d^3r \, \rho(r) \phi(r,t) \tag{36}$$

$$\frac{d}{d\lambda} W = -\frac{\hbar}{2}\frac{1}{Z}\underline{\frac{d}{d\lambda} Z}$$

$$\mathrm{tr}\left[\sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \int_p dt_1 \cdots \int_p dt_n \frac{d}{d\lambda} T_p\{[\lambda H_{1_{H_0}}(t_1) + \Phi_{H_0}(t_1)] \cdots\}\hat{\rho}\right]$$

$$= \mathrm{tr}\left[\sum_{n=1}^{\infty}\frac{1}{(n-1)!}\left(-\frac{i}{\hbar}\right)^n \int_p dt_1 \cdots \int_p dt_n T_p\{H_{1_{H_0}}(t_1)[\lambda H_{1_{H_0}}(t_2) + \Phi_{H_0}(t_2)] \cdots\}\hat{\rho}\right]$$

$$= -\frac{\cancel{\hbar}}{2}\left(-\frac{i}{\cancel{\hbar}}\right)\frac{1}{Z}\mathrm{tr}\{[T_p \int_p dt\, H_{1_{H_0}}(t_1) S_0]\hat{\rho}\}$$

$$\boxed{\therefore\ W - W_{\lambda=0} = \frac{i}{2}\int_0^1 d\lambda \int_p dt \langle H_1(t)\rangle_\lambda \quad (37)}$$

where

$$\langle O(t)\rangle = \mathrm{tr}\{T_p[O_{H_0}(t) S_0]\hat{\rho}\} / \mathrm{tr}(S_0\hat{\rho})$$

$$\xrightarrow[\phi=0]{} \mathrm{tr}\{T_p[O_{H_0}(t) S_0]\hat{\rho}\}|_{\phi=0} \quad (38)$$

Comparing Eqs. (34) and (37),

$$\boxed{A - A_{\lambda=0} = 2i(W - W_{\lambda=0}) \quad (39)}$$

§. Exchange-Correlation Action

The xc action is defined through

$$\boxed{A = \int_P dt \langle\Psi(t)|i\hbar\partial/\partial t - T|\Psi(t)\rangle_{\lambda=0} - n(\bar{1})v(\bar{1}) - \frac{1}{2}u(\bar{1},\bar{2})n(\bar{1})n(\bar{2}) - A_{xc}} \qquad (40)$$

Note that,

$$A_{\lambda=0} = \int_P dt \langle\Psi(t)|i\hbar\partial/\partial t - T|\Psi(t)\rangle_{\lambda=0} - n(\bar{1})v_{eff}(\bar{1}) \qquad (41)$$

Subtracting Eq. (41) from Eq. (40),

$$A - A_{\lambda=0} = n(\bar{1})\underbrace{[v_{eff}(\bar{1}) - v(\bar{1})]}_{w(\bar{1})} - \frac{1}{2}u(\bar{1},\bar{2})n(\bar{1})n(\bar{2}) - A_{xc} \qquad (42)$$

On the other hand, combining Eqs. (31) and (39),

$$A - A_{\lambda=0} = 2i\hbar\, \mathrm{tr}[\ln(G/G_0) - G_0^{-1}G + 1] + w(\bar{1})n(\bar{1}) - \frac{1}{2}u(\bar{1},\bar{2})n(\bar{1})n(\bar{2}) + 2i\,\Xi_{xc} \qquad (43)$$

Comparing Eqs. (42) and (43),

$$\boxed{A_{xc} = -2i\hbar\, \mathrm{tr}[\ln(G/G_0) - G_0^{-1}G + 1] - 2i\,\Xi_{xc}} \qquad (44)$$

§. Exchange-Correlation Potential

In Eq. (30),

$$\frac{\delta(W-W_{\lambda=0})}{\delta g(1',1)} = \hbar\underbrace{\left(\frac{\cancel{g_0}}{g}\frac{1}{\cancel{g_0}} - g_0^{-1}\right)} + \hbar\Sigma \quad = 0$$

From Eq. (18), $= -\Sigma$ for $\phi = 0$

$$\boxed{\therefore \quad \frac{\delta(W-W_{\lambda=0})}{\delta g(1',1)} = 0 = \frac{\delta(A-A_{\lambda=0})}{\delta g(1',1)} \qquad (45)}$$

Since the excess action does not depend on the change in g, A_{xc} does not too.

Now, consider the change δv_{eff}. From Eq. (19),

$$\delta g_0^{-1}(1,1') = -\hbar^{-1}\delta v_{eff}(1)\delta_p(1,1') \qquad (46)$$

Since A_{xc} depends only on the explicit change in g_0,

$$\delta A_{xc} = -2i\hbar\, \mathrm{tr}\ \frac{g_0}{\cancel{g}}\cdot\cancel{g}\cdot\delta g_0^{-1} - g\,\delta g_0^{-1}$$

$$= 2i\cancel{\hbar}\ \underbrace{[g(\bar{1}\bar{1}') - g_0(\bar{1}\bar{1}')]}_{\frac{i}{2}[n(\bar{1}) - n_0(\bar{1})]}\left(-\frac{1}{\cancel{\hbar}}\right)\delta v_{eff}(\bar{1})\delta_p(\bar{1}',\bar{1}')$$

$$= [n(\bar{1}) - n_0(\bar{1})]\,\delta v_{eff}(\bar{1})$$

From the definition, $n(1) = n_0(1)$, so that $\delta A_{xc} = 0$, i.e., A_{xc} does not depend on the change in $v_{eff}(r,t)$.

This δv_{eff} dependence may be rewritten by use of the Dyson equation,

$$0 = -2i \underbrace{[\mathcal{G}(\bar{1},\bar{1}^{+}) - \mathcal{G}_0(\bar{1},\bar{1}^{+})]}_{\mathcal{G}_0(\bar{1}\bar{2})\Sigma(\bar{2}\bar{3})\mathcal{G}(\bar{3}\bar{1}^{+})} \delta v_{eff}(\bar{1})$$

$$\boxed{\therefore \quad \mathcal{G}_0(1,\bar{2})\Sigma(\bar{2},\bar{3})\mathcal{G}(\bar{3},1) = 0 \qquad (47)}$$

Substituting Eq.(21) in Eq.(47),

$$\mathcal{G}_0(1,\bar{2})\left[\Sigma_{xc}(\bar{2},\bar{3}) - \hbar^{-1} v_{xc}(\bar{2},\bar{3})\,\delta_p(\bar{2},\bar{3})\right]\mathcal{G}(\bar{3},1) = 0$$

$$\boxed{v_{xc}(\bar{2})\mathcal{G}_0(1,\bar{2})\mathcal{G}(\bar{2},1) = \hbar\, \mathcal{G}_0(1,\bar{2})\Sigma_{xc}(\bar{2},\bar{3})\mathcal{G}(\bar{3},1) \qquad (48)}$$

※ Note that the functional derivative of A_{xc} with respect to $\delta v_{eff}(1)$ on the closed time path, not to the physical derivative

$$\delta f = \int_{-\infty}^{\infty} d1 \left(\frac{\delta f}{\delta v_{eff}^{+}(1)} - \frac{\delta f}{\delta v_{eff}^{-}(1)} \right)\Bigg|_{v_{eff}^{\pm}(1) = v_{eff}(1)} \delta v_{eff}(1),$$

because only $v_{eff}^{+}(1)$ is physically meaningful as a definition of the extended action, Eq.(34).

Generating Functional and Transformation Function

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$$\mathcal{H}(t) = H(t) + V(t) \tag{1}$$

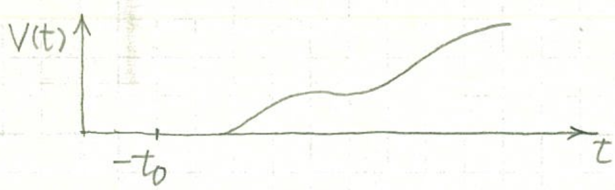
(Schrödinger Picture)

$$\begin{cases} |\Psi_S(t)\rangle = \mathcal{U}_\pm(t,t')\,|\Psi_S(t')\rangle \qquad (t \gtrless t') & (2) \\[1em] \mathcal{U}_\pm(t,t') = T_\pm \exp\left[-\frac{i}{\hbar}\int_{t'}^{t} dt_1\, \mathcal{H}(t_1)\right] & (3) \end{cases}$$

(Interaction Picture)

$$\begin{cases} |\Psi_H(t)\rangle = \mathcal{U}_-^H(-t_0,t)\,|\Psi_S(t)\rangle & (4) \\[1em] \mathcal{O}_H(t) = \mathcal{U}_-^H(-t_0,t)\,\mathcal{O}_S\,\mathcal{U}_+^H(t,-t_0) & (5) \end{cases}$$

$$\mathcal{U}_\pm^H(t,t') = T_\pm \exp\left[-\frac{i}{\hbar}\int_{t'}^{t} dt_1\, H(t_1)\right] \tag{6}$$

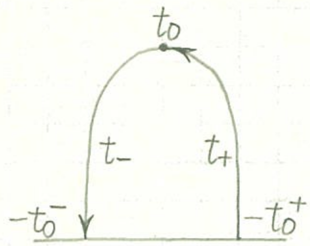


Then,

$$\begin{cases} |\Psi_H(t)\rangle = S_\pm(t,t')\,|\Psi_H(t')\rangle \qquad (t \gtrless t') & (7) \\[1em] S_\pm(t,t') = T_\pm \exp\left[-\frac{i}{\hbar}\int_{t'}^{t} dt_1\, V_H(t_1)\right] & (8) \end{cases}$$

§. Generating Functional

(Closed Time Path)



$$Z = \mathrm{tr}\,(\rho S)$$

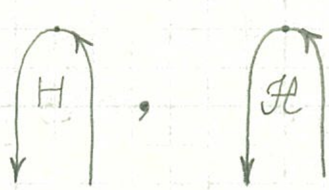
$$= \sum_i \rho_i \,\langle i| \underbrace{S(-t_0^-, -t_0^+)\,|i\rangle}$$

$$|i_I(-t_0^-)\rangle = \mathcal{U}_H^+(-t_0^+, -t_0^-)\,|i_S(-t_0^-)\rangle$$

$$= \sum_i \rho_i \,\langle i|\, \mathcal{U}_H^+(-t_0^+, -t_0^-)\,\mathcal{U}(-t_0^+, -t_0^-)\,|i\rangle$$

$$= \sum_i \rho_i \,(\, \mathcal{U}_H(-t_0^-, -t_0^+)\,\psi_i \,,\; \mathcal{U}(-t_0^-, -t_0^+)\,\psi_i\,)$$

$$\boxed{\begin{aligned} Z &\equiv \mathrm{tr}\,(\rho S) && (9)\\ &= \sum_i \rho_i\,(\mathcal{U}_H(-t_0^-, -t_0^+)\,\psi_i \,,\; \mathcal{U}(-t_0^-, -t_0^+)\,\psi_i\,) && (10)\end{aligned}}$$

Z = overlap ()

§. Transformation Function

$$\mathcal{T} \equiv \mathrm{tr}\,(\rho\,\mathcal{U}) \tag{11}$$

$$= \sum_i \rho_i \, \langle i | T \exp[-\tfrac{i}{\hbar}\int_p dt\, \mathcal{H}(t)] | i \rangle \tag{12}$$

§. Relation between Generating Functional and Transformation Function

$$Z = \sum_i \rho_i \, e^{i(\epsilon_i^+ - \epsilon_i^-)2t_0/\hbar} \, (\psi_i, \, \mathcal{U}(-t_0^-, -t_0^+)\, \psi_i) \tag{13}$$

for time independent H.

Further for $H_+ = H_-$ (however, still $\mathcal{H}_+ \neq \mathcal{H}_-$),

$$Z = \sum_i \rho_i \, (\psi_i, \, \mathcal{U}(-t_0^-, -t_0^+)\, \psi_i) = \mathcal{T} \tag{14}$$