Non-equilibrium quantum theory

(Rammer & Smith Rev. Mod. Phys
Kamenev book

Many-body field theory for time-dependent Hamiltonian $\underline{H(t)}$

Suppose we knew everything about the system at some distant past so at $t=-\infty$ the system is characterized by the known density matrix $\rho(-\infty)$. We use Heisenberg picture which refers to the state vector at ~~$-\infty$~~ $t=-\infty$!

$$\Rightarrow \quad \frac{\partial\rho}{\partial t} = -i\,[H,\rho] \qquad (\text{we use } \hbar = 1)$$

Heisenberg equation of motion

$$\rho(t) = U_{t,-\infty}\,\hat{\rho}(-\infty)\left[U_{t,-\infty}\right]^{+} = U_{t,-\infty}\,\hat{\rho}(-\infty)\,U_{-\infty,t}$$

where $U_{t,t'} = T\exp\left(-i\int_{t'}^{t} H(\tau)\,d\tau\right)$ — $\underline{\text{evolution operator}}$

deviation (The reminder on Schrödinger versus Heisenberg picture)

$\langle O \rangle = \langle \Psi_S | O_S | \Psi_S \rangle = \langle \Psi_H | O_H | \Psi_H \rangle$ – expectation value in quantum theory

Schrödinger picture:

$|\Psi_S(t)\rangle$ – time-dependent state vector: $i \frac{\partial |\Psi_S\rangle}{\partial t} = H_S |\Psi_S\rangle$

O_S – time-independent operator (observable)

Heisenberg picture:

$|\Psi_H\rangle$ – time-independent state vector, e.g. $|\Psi_H\rangle = |\Psi_S(t=-\infty)\rangle$

$$|\Psi_S\rangle = T\exp\left(-i\int_{-\infty}^{t} dt' H(t')\right)|\Psi_H\rangle = U_{t,-\infty}|\Psi_H\rangle$$

$$\langle O \rangle = \langle \Psi_H | \underbrace{\tilde{T}\exp\left(i\int_{-\infty}^{t} dt' H(t')\right)} O_S \underbrace{T\exp\left(-i\int_{-\infty}^{t} dt' H(t')\right)} |\Psi_H\rangle$$

anti-time ordering (earlier times on the left)

time ordering (earlier times on the right!)

$$\Rightarrow \quad O_H(t) = [U_{t,-\infty}]^\dagger O_S \, U_{t,-\infty} = U_{-\infty,t} O_S U_{t,-\infty}$$

~~time-independ~~

time-dependent operator $\qquad \dfrac{\partial O_H}{\partial t} = i[\mathcal{H}, O_H]$

In the simplest case $\rho(-\infty) = |\psi_H\rangle\langle\psi_H|$

In general $\rho(-\infty)$ describes statistical averaging $\hat\rho = e^{-\beta H}$

Quite generally $\langle O\rangle = \mathrm{Tr}\left(\hat\rho(t)\, O_{\mathcal{H}}(t)\right) / \mathrm{Tr}\,\hat\rho(t)$

$$= \mathrm{Tr}\left(\hat\rho(-\infty)\, U_{-\infty,t}\, O_{\mathcal{H}}(t)\, U_{t,-\infty}\right) / \mathrm{Tr}\,\hat\rho(t) \qquad \left(\mathrm{Tr}\,\rho(t) = \mathrm{Tr}\,\rho(-\infty)\right)$$

$\hat\rho(-\infty)$ describes known state at $t = -\infty$

If the state at $t=-\infty$ is unknown (e.g. due to interactions) we can always turn on the interactions as a function of time and anyway assume that the system is fully tractable at initial time $t = -\infty$

Traditional construction of zero temperature quantum-field theory

$|GS\rangle = U_{t,-\infty}|0\rangle$; $\langle GS|O|GS\rangle = \langle 0|U_{-\infty,t}\, O\, U_{t,-\infty}|0\rangle$

ground state

evolution operator $U_{t,-\infty}$ describes evolution of a simple non-interacting ground-state to $|GS\rangle$ upon <u>adiabatic switching</u> of interactions

Equilibrium trick : $\boxed{\text{Insert } U_{+\infty,-\infty}}$ i.e.

assume $\langle 0|U_{-\infty,t}\, O\, U_{t,-\infty}|0\rangle = \dfrac{\langle 0|U_{+\infty,-\infty}U_{-\infty,t}\, O\, U_{t,-\infty}|0\rangle}{\langle 0|U_{+\infty,-\infty}|0\rangle}$

In the other words one assumes that

$$\langle 0|U_{+\infty,-\infty} = \langle 0|\cdot \underbrace{e^{iL}}_{\text{phase factor}}$$

Adiabatic switching on & switching off interaction does not change the ground state! It only adds a phase factor!

Thus, one assumes in equilibrium theory

$$\langle GS | O | GS \rangle = \frac{\langle 0 | U_{+\infty, t} \, \hat{O} \, U_{t, -\infty} | 0 \rangle}{e^{iL}}$$

description of the evolution along the forward time axis

This comes with the price: (one has to take care of the denominator). This is, however, automatically cancelled by considering the so-called „connected" diagrams!

The trick $\langle 0 | U_{+\infty, -\infty} = \langle 0 | e^{iL}$ does not work in the non-equilibrium situation (i.e. for any non-adiabatic dependence on time in the Hamiltonian)

For real time dependence one cannot identify the states at $t = -\infty$ & at $t = +\infty$!

Non-equilibrium field theory

$$\langle O \rangle = \frac{\mathrm{Tr}\left(U_{-\infty,t}\, O_H(t)\, U_{t,-\infty}\, \rho(-\infty) \right)}{\mathrm{Tr}\, \rho(-\infty)} =$$

insert here $U_{t,+\infty}\, U_{+\infty,t} = 1$

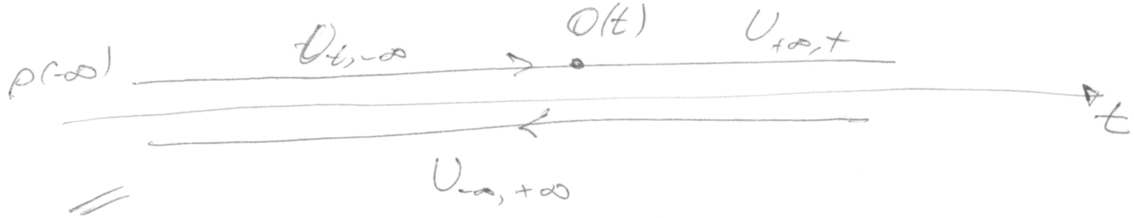
can also insert $U_{t,+\infty}\, U_{+\infty,t}$ between O_H and $U_{t,-\infty}$

$$= \frac{\mathrm{Tr}\left(U_{-\infty,+\infty}\, U_{+\infty,t}\, O\, U_{t,-\infty}\, \rho(-\infty) \right)}{\mathrm{Tr}\, \rho(-\infty)}$$

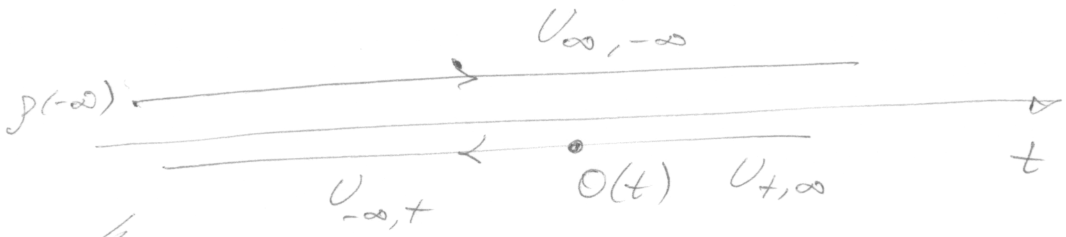
$$= \frac{\mathrm{Tr}\left(U_{-\infty,t}\, O\, U_{t,\infty}\, U_{\infty,-\infty}\, \rho(-\infty) \right)}{\mathrm{Tr}\, \rho(-\infty)}$$

It is convenient to take a half-sum of these two equivalent representations.

Keldysh contour:



$$\mathrm{Tr}\left(U_{-\infty,+\infty}\, U_{+\infty,t}\, O\, U_{t,-\infty}\, \rho(-\infty)\right)$$



$$\mathrm{Tr}\left(U_{-\infty,t}\, O\, U_{t,\infty}\, U_{\infty,-\infty}\, \rho(-\infty)\right)$$

Calculation of $\mathrm{Tr}\,\rho(-\infty)$ is never a problem!

It refers entirely to $\underline{t=-\infty}$

One can subsequently construct a field theory with a source term: $\hat{H}_0 = H(t) \pm O\,\eta(t)/2$

where + refers to the upper branch and − to lower branch of the contour. One can then define the generating functional $Z[\eta]$ as the trace of the evolution operator along the contour.

such that $\langle O \rangle = \left.\dfrac{\delta Z[\eta]}{\delta \eta(t)}\right|_{\eta=0}$ — functional derivative

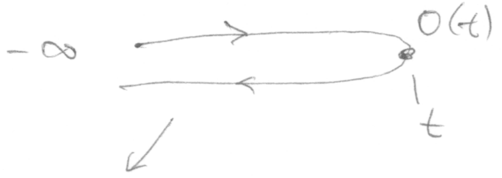
note that $Z[0] = 1$ - which greatly simplifies ~~the~~ such things like averaging over disorder. (In usual approach the phase factor e^{iL} depends on disorder realization, which makes the corresponding field theories very complex)

Once again:

$$\mathrm{Tr}\left(U_{-\infty,t}\, O\, U_{t,-\infty}\, \rho(-\infty)\right) = \mathrm{Tr}\left(\tilde{T}\exp\left(i\int_{-\infty}^{t} \mathcal{H}(\tau)\,d\tau\right) O\; T\exp\left(-i\int_{-\infty}^{t}\mathcal{H}(\tau)\,d\tau\right)\rho(-\infty)\right) =$$

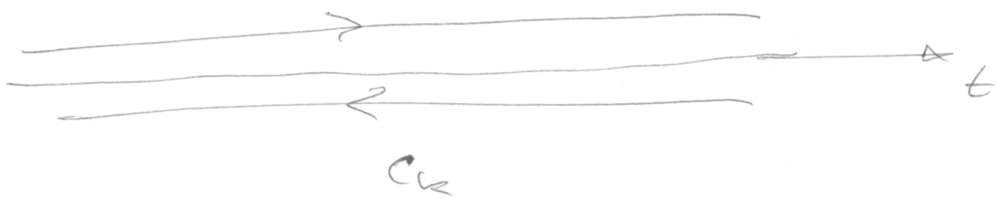
$$\equiv \mathrm{Tr}\left(T_C\left[\exp\left(-i\int_{C_t}\mathcal{H}(t)\,dt\right) O(t)\right]\rho(-\infty)\right)$$

time ordering on the contour



This can be equivalently written as the time-ordering along Keldysh contour with O placed either on the upper or on the lower branch:

$$\equiv \mathrm{Tr}\left(T_{C_K}\left[\exp\left(-i\int_{C_K}\mathcal{H}(\tau)\,d\tau\right) O(t)\right]\rho(-\infty)\right)$$



Non-equilibrium Green's functions

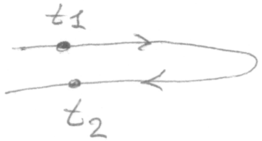
Expectation values of non-equilibrium theory can be expressed with the help of non-equilibrium Green's functions, that are defined as correlators on Keldysh contour:

for fermions: $G_{C_K}(1,2) = -i \langle T_{C_K}(\Psi(1)\, \Psi^\dagger(2)) \rangle$

time ordering on the contour

$1 \equiv \tau_1, t_1$
$2 \equiv \tau_2, t_2$ ← short-hand notations

we have 4 different possibilities to place t_1 & t_2 on the contour



$\Rightarrow$ t_2 is always larger (on the contour)

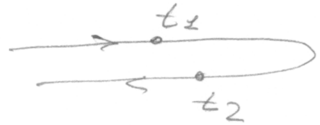
$$\Rightarrow \quad G \rightarrow G_{12}(1,2) \equiv G^<(1,2) = i \langle \Psi^\dagger(2)\, \Psi(1) \rangle$$

To summarize:

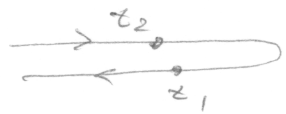
$$G_{C_K} = -i \langle T_{C_K} (\Psi(1) \Psi^\dagger(2)) \rangle \quad \Longrightarrow \quad \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix} (1,2)$$

represented by a matrix in Keldysh space

$$G^<(1,2) = G_{12}(1,2) = i \langle \Psi^\dagger(2) \Psi(1) \rangle$$

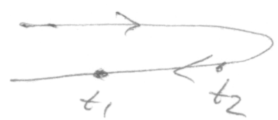


$$G^>(1,2) = G_{21}(1,2) = -i \langle \Psi(1) \Psi^\dagger(2) \rangle$$



$$G_{11}(1,2) = -i \langle T (\Psi(1) \Psi^\dagger(2)) \rangle = -i \theta(t_1 - t_2) \langle \Psi(1) \Psi^\dagger(2) \rangle + i \theta(t_2 - t_1) \langle \Psi^\dagger(2) \Psi(1) \rangle$$

$$G_{22}(1,2) = -i \langle \tilde{T} (\Psi(1) \Psi^\dagger(2)) \rangle = -i \theta(t_2 - t_1) \langle \Psi(1) \Psi^\dagger(2) \rangle + i \theta(t_1 - t_2) \langle \Psi^\dagger(2) \Psi(1) \rangle$$



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these 4 Green's functions are NOT linearly independent!

Prove that!

It is instructive to relate the Green's functions in Keldysh space

$$G^<(1,2) = G_{12}(1,2) = i\langle \psi^+(2)\psi(1)\rangle$$
$$G^>(1,2) = G_{21}(1,2) = -i\langle \psi(1)\psi^+(2)\rangle$$
$$G_{11}(1,2) = -i\langle T\,\psi(1)\psi^+(2)\rangle = -i\theta(t_1-t_2)\langle \psi(1)\psi^+(2)\rangle + i\theta(t_2-t_1)\langle \psi^+(2)\psi(1)\rangle$$
$$G_{22}(1,2) = -i\langle \tilde{T}\,\psi(1)\psi^+(2)\rangle = -i\theta(t_2-t_1)\langle \psi(1)\psi^+(2)\rangle + i\theta(t_1-t_2)\langle \psi^+(2)\psi(1)\rangle$$

to the following 3 Green's functions:

$$G^R(1,2) = -i\theta(t_1-t_2)\langle\{\psi(1),\psi^+(2)\}\rangle \quad \leftarrow \text{non-zero only for } t_1 \geq t_2 \text{ (retarded)}$$
$$G^A(1,2) = i\theta(t_2-t_1)\langle\{\psi(1),\psi^+(2)\}\rangle \quad \leftarrow \text{non-zero for } t_2 \geq t_1 \text{ (advanced)}$$
$$G^K(1,2) = -i\langle[\psi(1),\psi^+(2)]\rangle, \quad \{A,B\} \equiv AB+BA \;;\; [A,B] = AB-BA$$

G^R, G^A – contain information about the spectrum of the system!

G^K – contains in addition the information about occupation of the spectrum by quasiparticles.

In equilibrium, we never introduced G^K assuming that this occupation follows from Fermi & Bose distributions.

In non-equilibrium we have to solve some equation to find G^K and establish the occupation of the spectrum. In simple quasiclassical approximation this equation is reduced to Boltzmann equation.

The rotation

Linear dependence :
&
relation to linearly independent components

$$\begin{cases} \underbrace{G_{11}(1,2)+G_{22}(1,2) = G_{12}(1,2)+G_{21}(1,2)} = G^K(1,2) \\ G_{11}(1,2)-G_{22}(1,2) = G^R(1,2)+G^A(1,2) \\ G_{21}(1,2)-G_{12}(1,2) = G^R(1,2)-G^A(1,2) = -i\langle\{\psi(1),\psi^+(2)\}\rangle \end{cases}$$

Original keldysh space :

$$\underline{G} = \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix}$$

keldysh „rotation"

$$G = \hat{L}\,\tau_z\,\underline{G}\,\hat{L}^+ \quad , \quad \tau_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} , \quad L = \frac{1}{\sqrt{2}}(1-i\tau_y) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$$

$$\Rightarrow \quad G = L\begin{pmatrix} G_{11} & G_{12} \\ -G_{21} & -G_{22} \end{pmatrix} L^+ = \frac{1}{2}\begin{pmatrix} G_{11}-G_{22}+G_{21}-G_{12} \;, & G_{11}+G_{22}+G_{12}+G_{21} \\ G_{11}+G_{22}-G_{12}-G_{21} \;, & G_{11}-G_{22}+G_{12}-G_{21} \end{pmatrix} = \begin{pmatrix} G^R & G^K \\ 0 & G^A \end{pmatrix}$$

$$\Rightarrow \quad G_{11} = \frac{1}{2}\left(G^K+G^R+G^A\right) \quad , \quad G_{12} = \frac{1}{2}\left(G^K-G^R+G^A\right)$$

$$G_{21} = \frac{1}{2}\left(G^K+G^R-G^A\right) \quad , \quad G_{22} = \frac{1}{2}\left(G^K-G^R-G^A\right)$$

Dyson equation (perturbation to anything)

Perturbation to external potential $\qquad \mathcal{H} = H_0 + V(r,t)$

$$G_{ck}(1,2) = -i \langle T_{ck}\, \psi(1)\, \psi^+(2) \rangle$$

$$\Rightarrow \quad \underbrace{(i\partial_{t_1} - \mathcal{H}_1)}_{\text{operator acting on } t_1, r_1} G_{ck}(1,2) = \delta(1-2) \;\; \text{(}\equiv \delta(t_1-t_2)\,\delta^{(3)}(r_1-r_2)\text{)}$$

first order perturbation

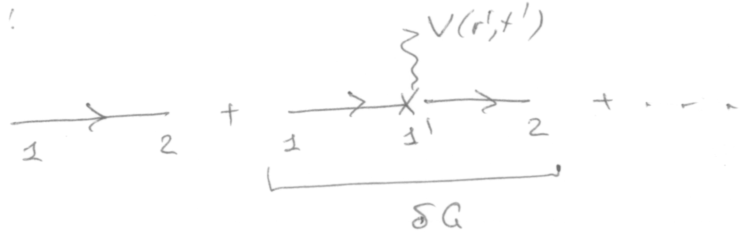
$$\Rightarrow \quad G_{ck}(1,2) = G^{(0)}_{ck}(1,2) + \underbrace{\int G^{(0)}_{ck}(1,1')\, \underbrace{V(1')}_{\text{local}}\, G^{(0)}_{ck}(1',2)\, d1'}_{\equiv\, \delta G}$$

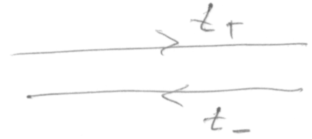
$d1'$: convolution in space and Keldysh time

$$\Rightarrow \quad \delta G = \int_{ck} dt' \int d^3r'\, G^{(0)}_{ck}(t_1, r_1; t', r')\, V(t', r')\, G^{(0)}_{ck}(t', r'; t_2\, r_2)$$

we assume convolution in r (but often do not write it explicitely)

Diagrams:

$G(1,2) =$ 



$$\delta G_{C_K}(1,2) = \int_{C_K} dt'\, G^{(0)}(t_1,t')\, V(t')\, G^{(0)}(t',t_2) = \left(\int_{-\infty}^{+\infty} dt'_+ - \int_{-\infty}^{+\infty} dt'_-\right) G^{(0)} V G^{(0)}$$

$\Downarrow$ to keldysh space: $\begin{pmatrix} 1\in t_+\ 2\in t_+ , & 1\in t_+ , 2\in t_- \\ 1\in t_- , 2\in t_+ , & 1\in t_-\ 2\in t_- \end{pmatrix}$

$$\underline{\delta G} = \int_{-\infty}^{+\infty} dt'\, \underbrace{\underline{G}^{(0)}(t_1,t')}_{\text{matrix}}\, \underline{V}(t')\, \underbrace{\tau_z}_{\text{takes care of "-" for lower branch}}\, \underline{G}^{(0)}(t',t_2) \quad \leftarrow \underline{\text{check that}}!$$

$$\underline{V} = \begin{pmatrix} V_+ & 0 \\ 0 & V_- \end{pmatrix} \qquad \begin{aligned} V_+ &= V(t'_+) \\ V_- &= V(t'_-) \end{aligned}$$

$\Downarrow$ keldysh rotation

$$\hat{\delta G} = L\tau_z \underline{\delta G} L^+ = L\tau_z G^{(0)} \underline{V} \tau_z G^{(0)} L^+ = \overbrace{\underbrace{L\tau_z \underline{G}^{(0)} L^+}} L(\underline{V}\tau_z)\, \underbrace{\tau_z L^+ L \tau_z}_{1} \overbrace{\underline{G}^{(0)} L^+}$$

$$= \hat{G}^{(0)} L V L^+ \hat{G}^{(0)}$$

$$L V L^+ = L \begin{pmatrix} V_+ & 0 \\ 0 & V_- \end{pmatrix} L^+ = \hat{1}\, \underbrace{\frac{V_+ + V_-}{2}}_{V_{cl}} + \tau_x \underbrace{\frac{V_+ - V_-}{2}}_{V_q}$$

For classical potential

$V_+ = V_- = V$

V_q - quantum fluctuation

External potential is describing also practically any interaction

$\Rightarrow \quad \mathcal{H}_{int} = g \int d^2r \; \psi^+(r,t)\, \psi(r,t)\, \underbrace{\varphi(r,t)}_{\text{bosonic field}}$

Is φ is quantum field then φ_q is very important!!

We come to this later.

$$\boxed{\text{Wigner transform}}$$ ← another central concept

$$G(t_1, \vec{r}_1 ; t_2, \vec{r}_2) = \int \frac{d\varepsilon}{2\pi} e^{-i\varepsilon(t_1 - t_2)} \int \frac{d^3p}{(2\pi)^3} e^{i\vec{p}\cdot(\vec{r}_1 - \vec{r}_2)} \underline{G(\varepsilon, T; \vec{p}, \vec{R})}$$

Wigner transform with respect to time

Wigner transform with respect to space

ie independent variables

$T = \frac{t_1 + t_2}{2}, \quad R = \frac{r_1 + r_2}{2}$

Wigner-transform

$G(\varepsilon, T; p, R)$ – smooth function of all variables!

T – physical time

R – physical coordinate

ε – energy

p – momentum

In full equilibrium: $\underline{G(\varepsilon, T; p, R) = G(\varepsilon, p)}$

both in time & in „space"

In equilibrium (with respect to time)

$$\boxed{G^K(\varepsilon; r_1, r_2) = \tanh\frac{\varepsilon}{2T}\left(G^R(\varepsilon; r_1, r_2) - G^A(\varepsilon; r_1, r_2)\right)}$$

fluctuation-dissipation theorem

does not require space equilibrium

<u>Prove it later!</u>

translational invariance in time $\Rightarrow$ time equilibrium

translational invariance in space $\Rightarrow$ space equilibrium
(usually absent apart from clean infinite systems)

$\cancel{G^>(1,2) = -i\langle\psi(1)\psi^\dagger(2)\rangle}$ $\quad G^<(1,2) = i\langle\psi^\dagger(2)\,\psi(1)\rangle$

~~At~~ Expectation values in non-equilibrium for single-particle operators:

e.g. $\hat{j}$ - current operator $\quad \cancel{\langle \hat j\rangle = -i\,\mathrm{Tr}\,\hat j}$

coinciding arguments ~~(...)~~

$$\langle \hat j\rangle = -i\,\cancel{\mathrm{Tr}}\,\hat j\, G^<(r,t; r,t) = \langle \underline{\psi_t^\dagger\, \hat j\, \psi_t}\rangle$$

(see below for details)

Since most of interesting operators are single-particle operators we can already make lots of interesting predictions!

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deviation ; a reminder concerning current operator for simple model of non-relativistic electrons

$$H = \frac{\hat{p}^2}{2m} + \hat{V} \to \frac{(\hat{p} - eA)^2}{2m} + V(r) \;, \quad \hat{p} = -i\vec{\nabla} \qquad (\hbar = 1)$$

in second quantization : $H = \int d^3r \; \hat{\Psi}^+(r,t) \frac{1}{2m} \left(\hat{p} - e\vec{A}(r,t)\right)^2 \hat{\Psi}(r,t)$

vector potential

$$\hat{j} = -\frac{\delta \hat{H}}{\delta A(r,t)} \; ;$$

$$H = \int dr \left(\psi^+ \frac{p^2}{2m} \psi + \frac{e}{2m} (\hat{p}\psi^+) \psi A - \frac{e}{2m} \psi^+ (p\psi) A + \frac{e^2}{2m} |A|^2 \psi^+ \psi \right)$$

$$\hat{j} = -\left(-\frac{ie}{2m} (\nabla\psi^+)\psi + \frac{ie}{2m} \psi^+ (\nabla\psi) + \frac{e^2}{m} \vec{A} |\psi|^2 \right) \leftarrow$$ current in second quantization

$\Downarrow$

single particle operator : $\boxed{\hat{j} = -\frac{ie}{2m} (\vec{\nabla} - \overleftarrow{\nabla}) - \underbrace{\frac{e^2}{m} \vec{A}}}$

diamagnetic term