Lecture on First-principles Computations (23) the Feynman Diagrams and the Self-energy

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Green function in the interaction picture

$$G(x,x';t-t') = -i\frac{\langle\Psi_0 \mid \hat{T}\left[\hat{\psi}_H(x,t)\hat{\psi}_H^\dagger(x',t')\right] \mid \Psi_0\rangle}{\langle\Psi_0 \mid \Psi_0\rangle} = \frac{-i}{\langle\Phi_0 \mid \hat{S}(\infty,-\infty) \mid \Phi_0\rangle}\times$$

$$\langle\Phi_0 \mid \sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} d\,t_n \hat{T}\left[\hat{H}_{int}(t_1)\cdots\hat{H}_{int}(t_n)\hat{\psi}_I(x,t)\hat{\psi}_I^\dagger(x',t')\right] \mid \Phi_0\rangle$$

The numerator

$$\tilde{G}(x,x';t-t') = -i\langle\Psi_0 \mid \hat{T}\left[\hat{\psi}_H(x,t)\hat{\psi}_H^\dagger(x',t')\right] \mid \Psi_0\rangle =$$

$$-i\,\langle\Phi_0 \mid \sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} d\,t_n \hat{T}\left[\hat{H}_{int}(t_1)\cdots\hat{H}_{int}(t_n)\hat{\psi}_I(x,t)\hat{\psi}_I^\dagger(x',t')\right] \mid \Phi_0\rangle$$

The denominator

$$\langle\Phi_0 \mid \hat{S}(\infty,-\infty) \mid \Phi_0\rangle = \langle\Phi_0 \mid \sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} d\,t_n \hat{T}\left[\hat{H}_{int}(t_1)\cdots\hat{H}_{int}(t_n)\right] \mid \Phi_0\rangle$$

The first few terms of $\tilde{G}(x, x'; t - t')$

- The zeroth-order term (non-interacting Green function):

$$\tilde{G}^{n=0}(x, x'; t - t') = -i\langle \Phi_0 \mid \hat{T}\left[\widehat{\psi}_I(x, t)\widehat{\psi}_I^{\dagger}(x', t')\right] \mid \Phi_0 \rangle = G_0(x, x'; t - t')$$

- The first-order term

$$\tilde{G}^{n=1}(x, x'; t - t') = -\langle \Phi_0 \mid \int_{-\infty}^{\infty} dt_1\, \hat{T}\left[\widehat{H}_{int}(t_1)\widehat{\psi}_I(x, t)\widehat{\psi}_I^{\dagger}(x', t')\right] \mid \Phi_0 \rangle$$

$$= -\frac{1}{2}\int_{-\infty}^{\infty} dt_1 \int d\,x_1 \int d\,x_2 V(x_1 - x_2) \times$$

$$\langle \Phi_0 \mid \hat{T}\left[\widehat{\psi}^{\dagger}(x_{1,}t_1)\widehat{\psi}^{\dagger}(x_{2,}t_1)\widehat{\psi}(x_{2,}t_1)\widehat{\psi}(x_{1,}t_1)\widehat{\psi}(x, t)\widehat{\psi}^{\dagger}(x', t')\right] \mid \Phi_0 \rangle$$

Six terms (3!) according to the Wick theorem!

- The second-order has 120 (5!) expansion terms

The 6 terms of $\tilde{G}^{n=1}(x, x'; t - t')$

$$\tilde{G}^{n=1}(x, x'; t-t') = -\frac{1}{2}\int_{-\infty}^{\infty} dt_1 \int d\,x_1 \int d\,x_2 V(x_1 - x_2)[(1) + (2) + (3) + (4) + (5) + (6)]$$

$$(1) = \left(-iG_0\left(x_{1,}x_1; 0^-\right)\right)\left(-iG_0\left(x_{2,}x_2; 0^-\right)\right)\left(iG_0(x, x'; t-t')\right)$$

$$(2) = -\left(-iG_0\left(x_{1,}x_2; 0^-\right)\right)\left(-iG_0\left(x_{2,}x_1; 0^-\right)\right)\left(iG_0(x, x'; t-t')\right)$$

$$(3) = -\left(-iG_0(x, x_1; t-t_1)\right)\left(-iG_0\left(x_{2,}x_2; 0^-\right)\right)\left(iG_0\left(x_{1,}x'; t_1-t'\right)\right)$$

$$(4) = \left(-iG_0\left(x_{1,}x_2; 0^-\right)\right)\left(-iG_0(x, x_1; t-t_1)\right)\left(iG_0\left(x_{2,}x'; t_2-t'\right)\right)$$

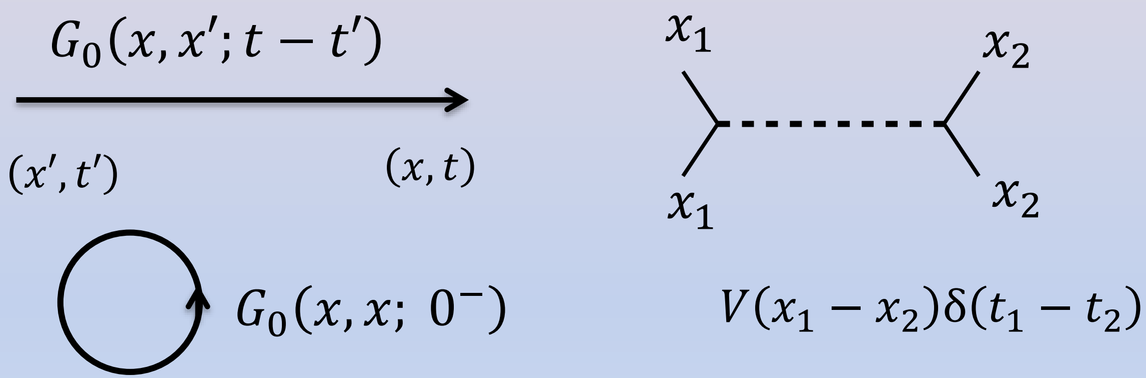
$$(5) = -\left(-iG_0(x, x_2; t-t_1)\right)\left(-iG_0\left(x_{1,}x_1; 0^-\right)\right)\left(iG_0\left(x_{2,}x'; t_1-t'\right)\right)$$

$$(6) = \left(-iG_0\left(x_{2,}x_1; 0^-\right)\right)\left(-iG_0(x, x_2; t-t_1)\right)\left(iG_0\left(x_{1,}x'; t_2-t'\right)\right)$$

Lengthy and non-intuitive!

The way out: Feynman diagrams

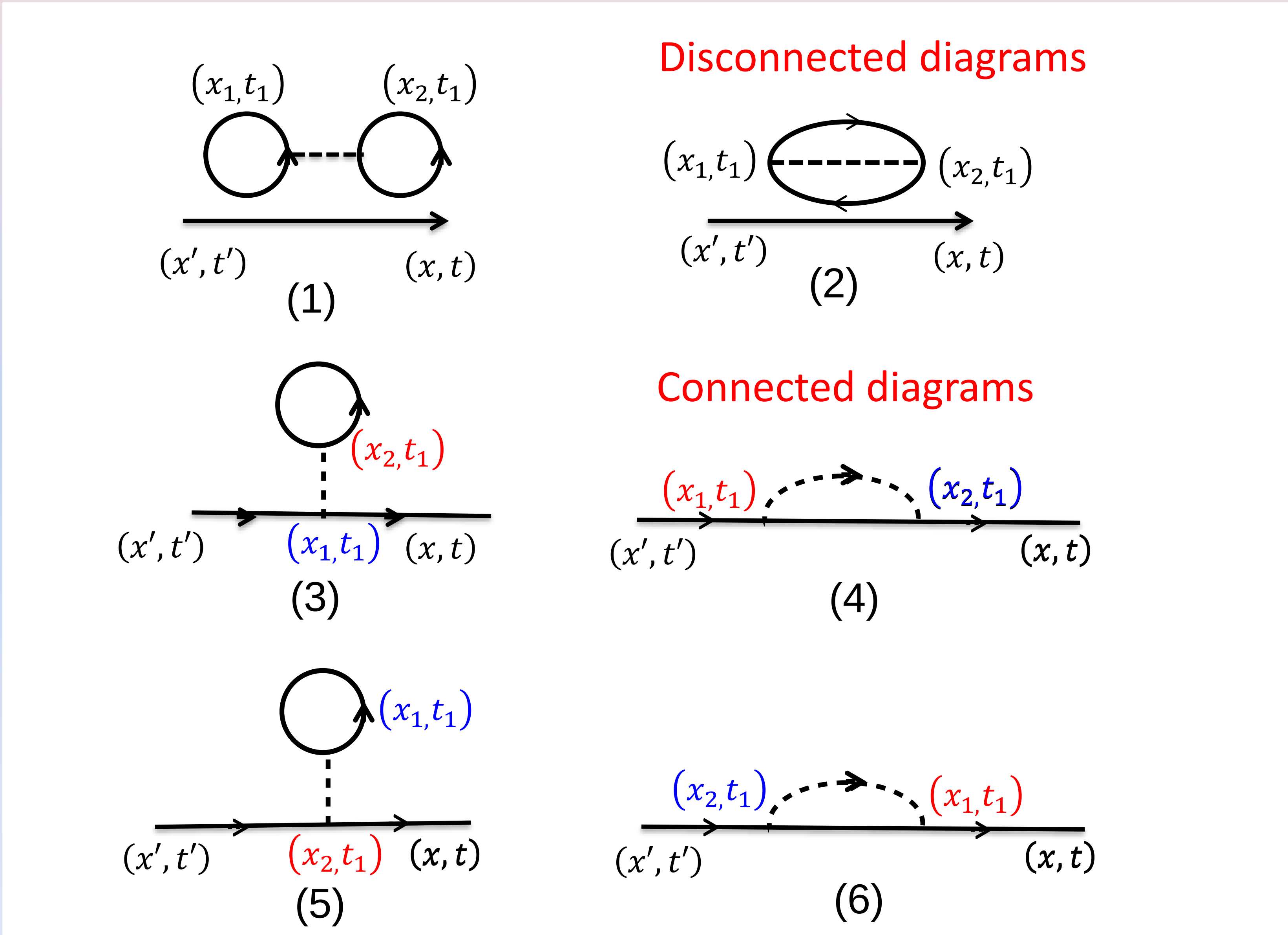
Using pictures to represent the algebraic expressions!



Advantages of Feynman diagrams:

- Intuitive, and reflects the underlying physical processes
- Reveals simple rules for accounting for physically relevant contributions.

Feynman diagrams for the first-order terms



The cancellation theorem

The Green function in the numerator $\tilde{G}$ factorizes into connected and disconnected parts !

$$\tilde{G}(x,x';t-t') = -i\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}dt_1\cdots\int_{-\infty}^{\infty}d\,t_n$$
$$\times\langle\Phi_0\mid\hat{T}\left[\hat{H}_{int}(t_1)\cdots\hat{H}_{int}(t_n)\hat{\psi}_I(x,t)\hat{\psi}_I^{\dagger}(x',t')\right]\mid\Phi_0\rangle_{\text{connected}}$$
$$\times\langle\Phi_0\mid S(\infty,-\infty)\mid\Phi_0\rangle$$

The closed part of disconnected diagrams

The true Green function:

$$G(x,x';t-t') = \frac{\tilde{G}(x,x';t-t')}{\langle\Phi_0\mid S(\infty,-\infty)\mid\Phi_0\rangle} = -i\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}dt_1\cdots\int_{-\infty}^{\infty}d\,t_n$$
$$\times\langle\Phi_0\mid\hat{T}\left[\hat{H}_{int}(t_1)\cdots\hat{H}_{int}(t_n)\hat{\psi}_I(x,t)\hat{\psi}_I^{\dagger}(x',t')\right]\mid\Phi_0\rangle_{\text{connected}}$$

Only connected diagrams need to be taken into account!

The counting factor

For each connected diagram at order *n*, there are $2^n n!$ many diagrams that have the same "topological structure". They differ only in the permutation of the dummy integration variables, and hence yield the same contribution! Killing the $1/n!$ prefactor (and also 2^n from the Coulomb interaction).

Only topologically different connected diagrams need to be taken into account!

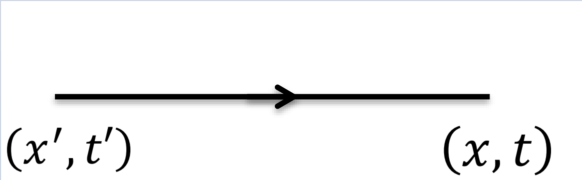
- For $n=1$, the number of topologically different connected diagrams is 2.
- For $n=2$, this number is 10. (Remember the total number is $5! = 120$)

Perturbation expansion for the Green function

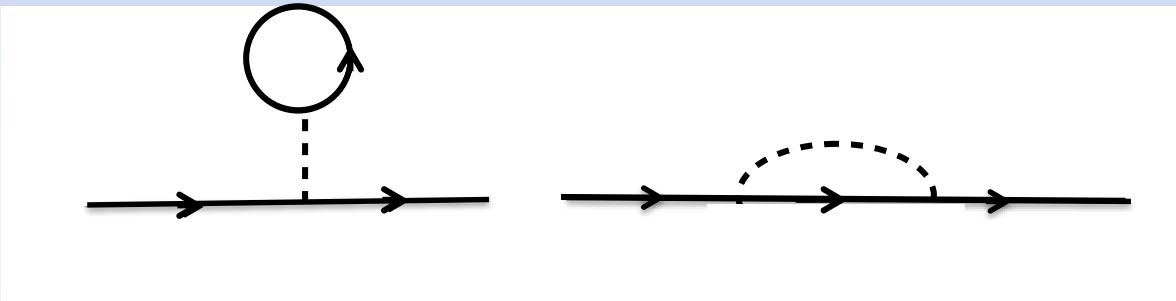
$$G(x,x';t-t') = -i\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}dt_1\cdots\int_{-\infty}^{\infty}d\,t_n$$
$$\times\langle\Phi_0 \mid \hat{T}\left[\hat{H}_{int}(t_1)\cdots\hat{H}_{int}(t_n)\hat{\psi}_I(x,t)\hat{\psi}_I^{\dagger}(x',t')\right] \mid \Phi_0\rangle_{\text{connected}}$$

- The zeroth order :

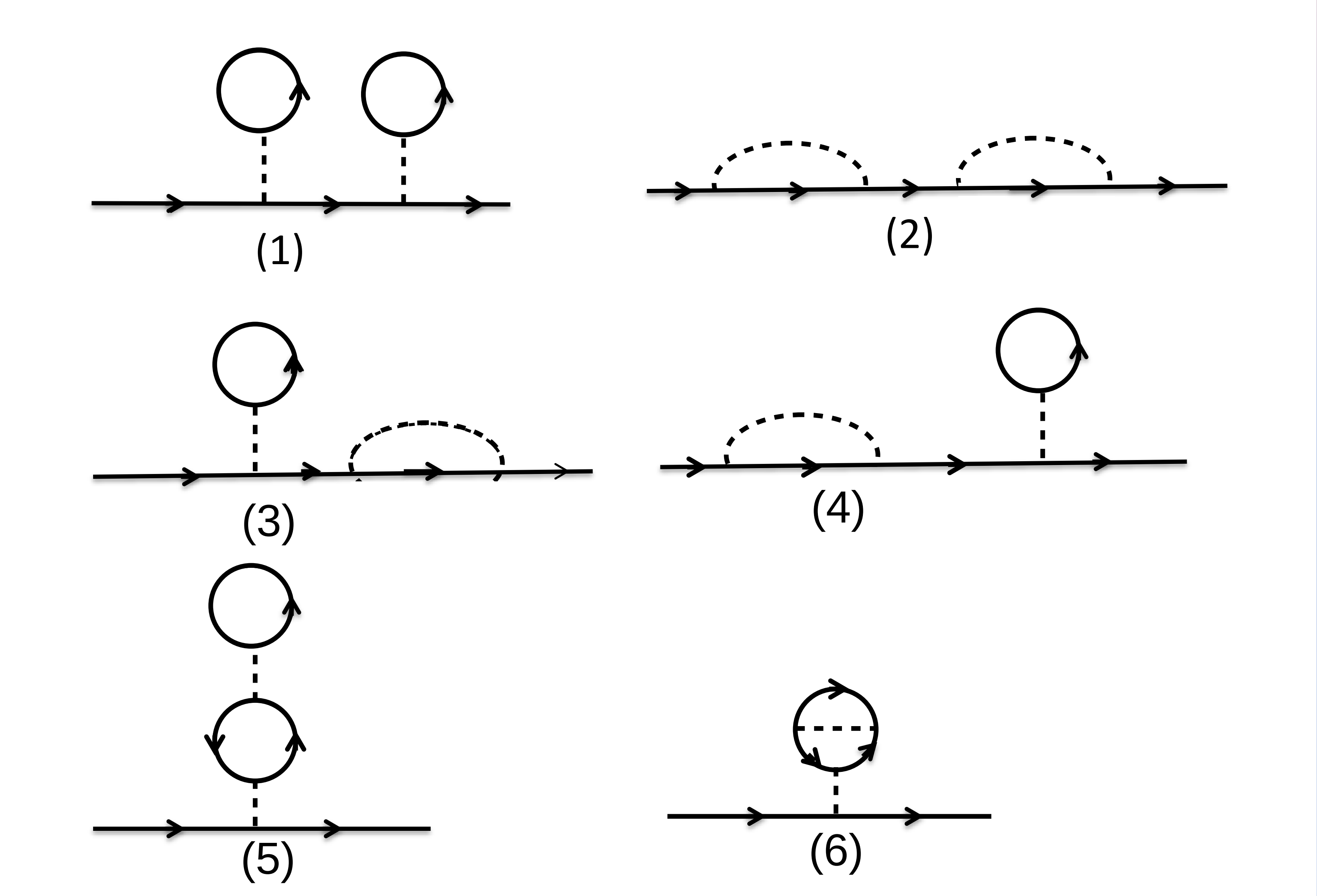
$G^0(x,x';t-t')$



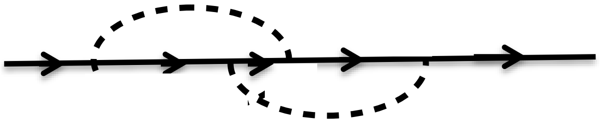
- The first order



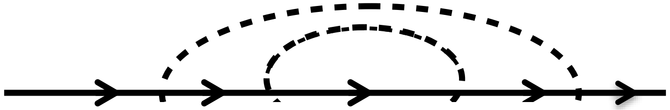
The second-order diagrams



The second-order diagrams (continued)



(6)



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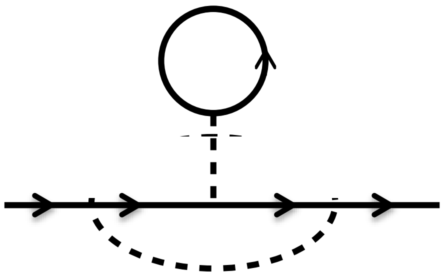

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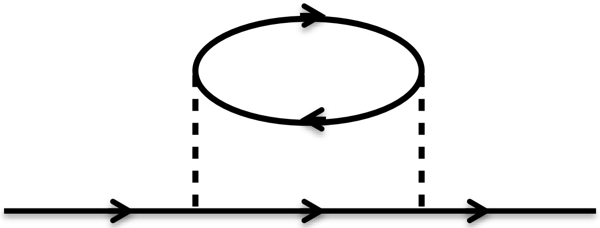
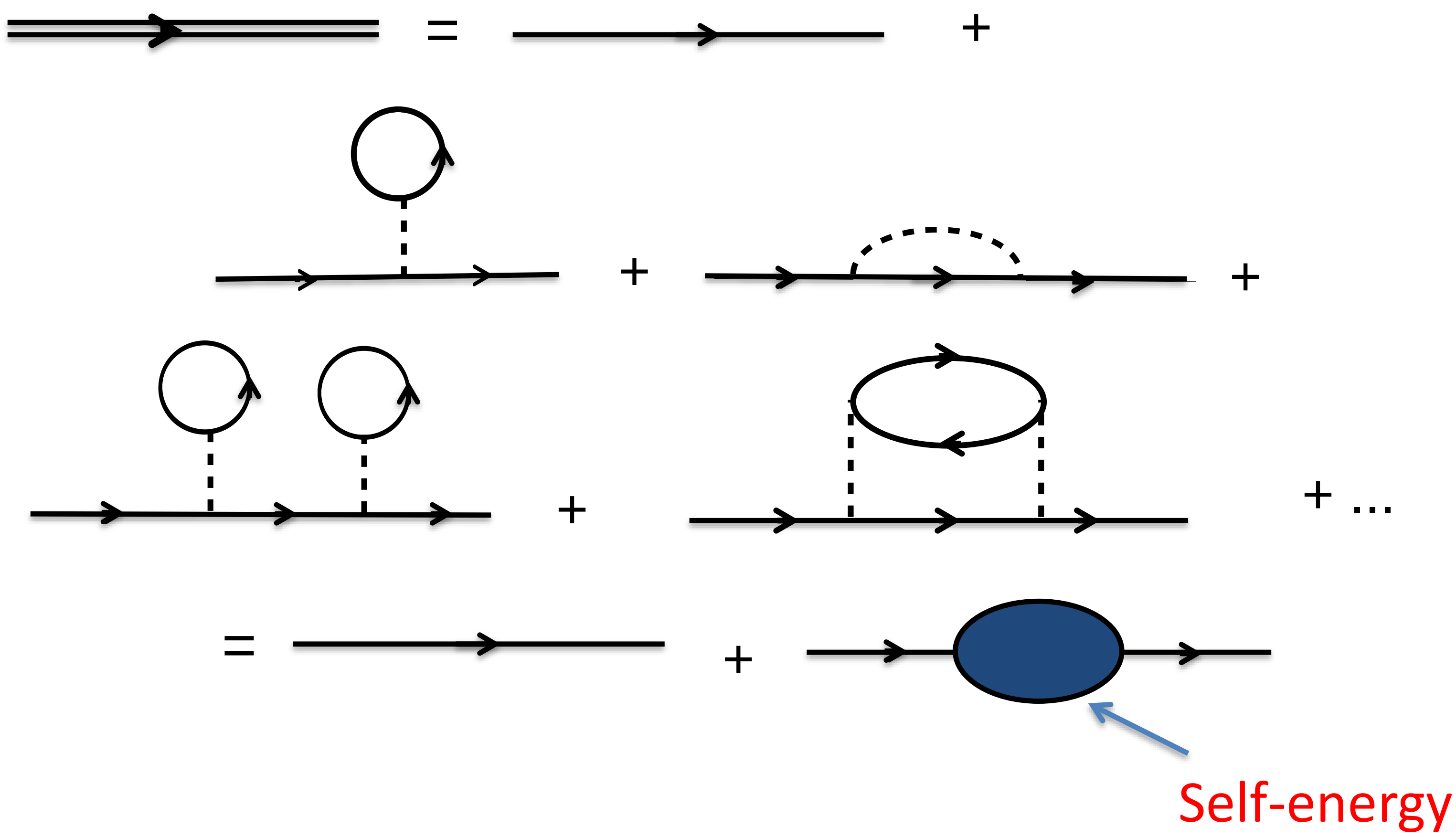
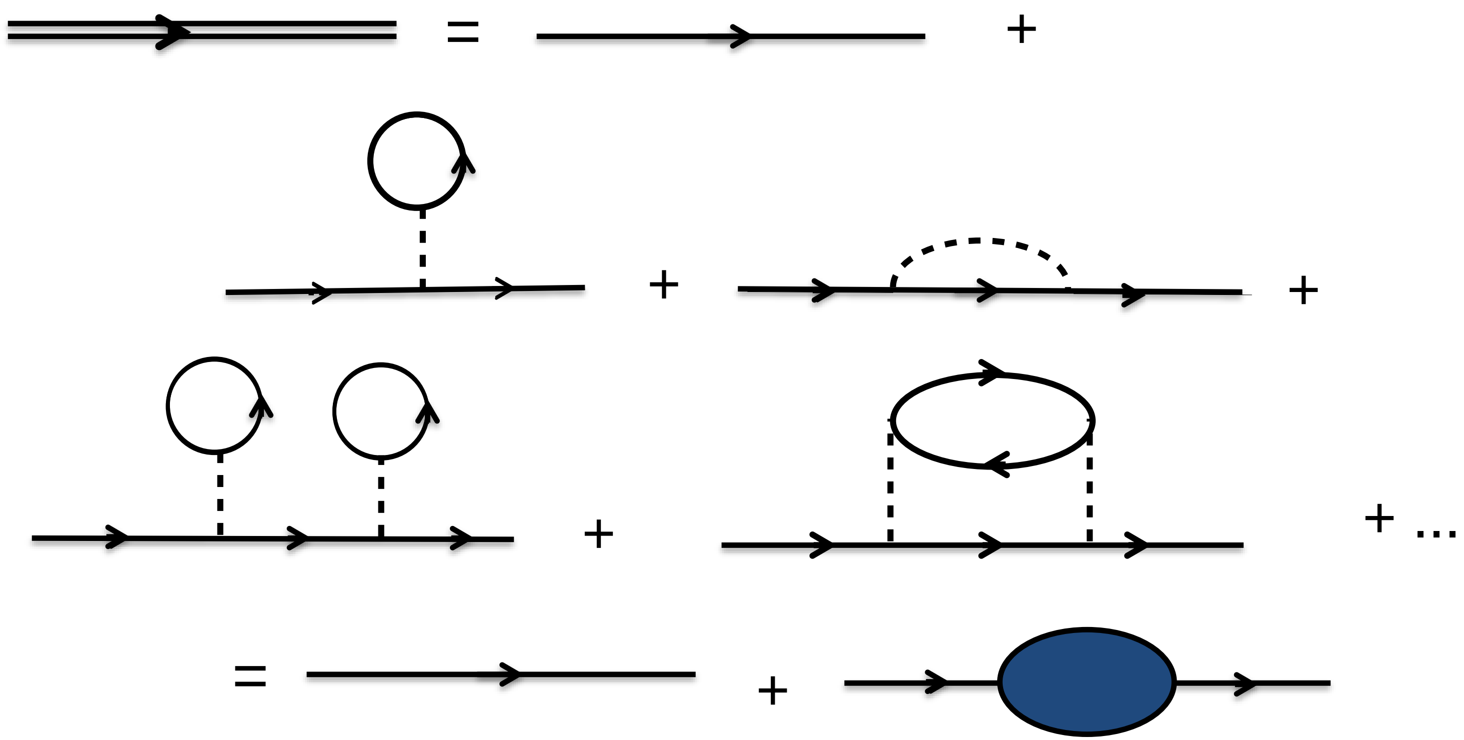


(10)

The self-energy



The self-energy

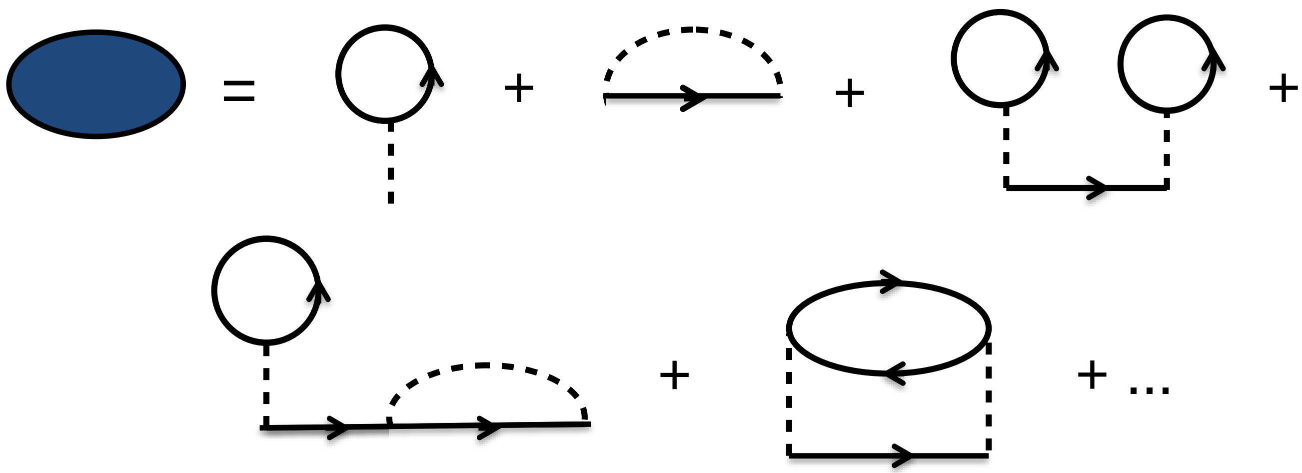


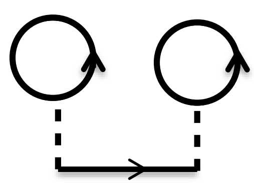
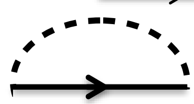
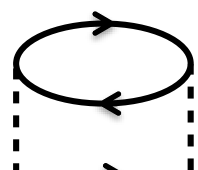
$$G(x,x';t-t') = G_0(x,x';t-t') + \int dx_1\, dx_2 dt_1 dt_2 G_0(x,x_1;t-t_1)\Sigma\big(x_1,x_2;t_1-t_2\big)G_0\big(x_2,x';t_2-t'\big)$$

The proper and improper self-energy terms

Fourier transform to the frequency domain:

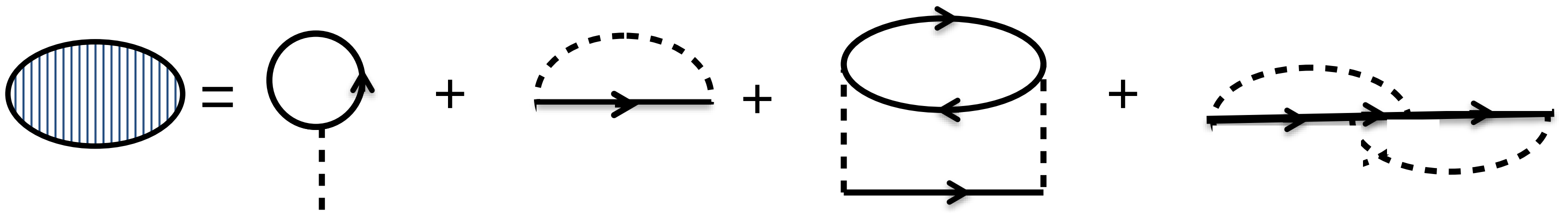
$$G(x,x';\omega) = G_0(x,x';\omega) + \int dx_1\, dx_2 G_0(x,x_1;\omega)\Sigma(x_{1,}x_2;\omega)G_0(x_{2,}x';\omega)$$



- Improper self-energy:  (can be broken into two pieces by cutting a single line)
- Proper self-energy  

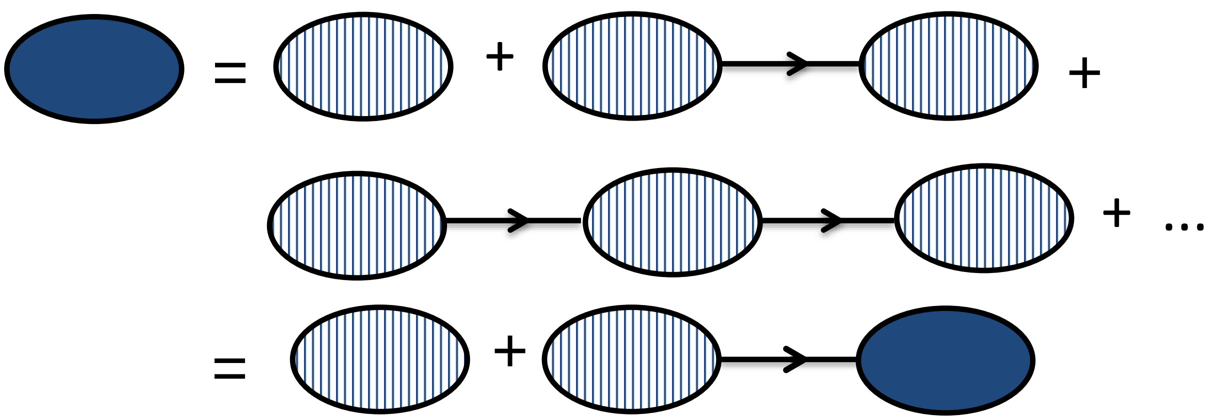
The structure of the self-energy

Define the total proper self-energy (Σ^*):



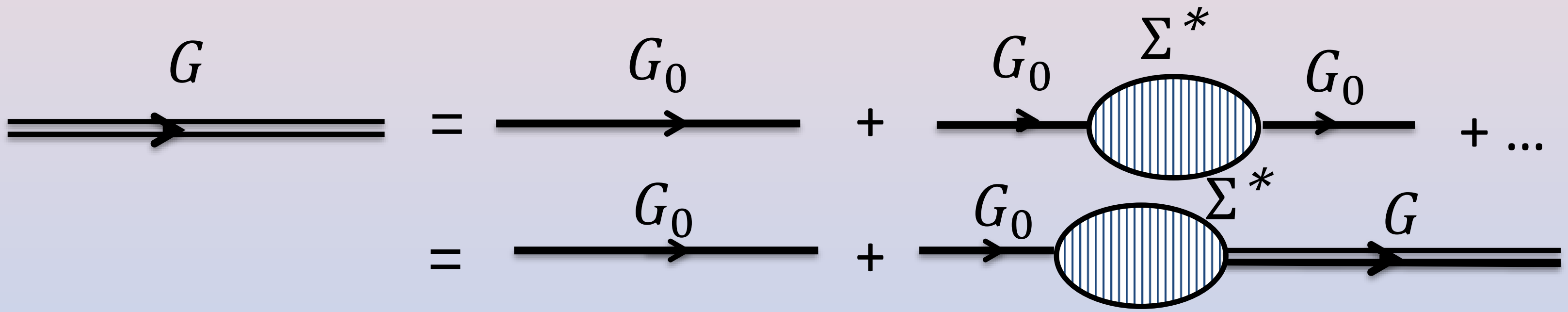
+ (all proper self-energy diagrams)

Dyson showed:



$$\Sigma = \Sigma^* + \Sigma^* G_0 \Sigma$$

Dyson equation



$$\left.\begin{aligned} \Sigma &= \Sigma^* + \Sigma^* G_0 \Sigma \\ G &= G_0 + G_0 \Sigma G_0 \end{aligned}\right\}$$

➡ Dyson equation

$$G = G_0 + G_0\Sigma^* G_0 + G_0\Sigma^* G_0\Sigma^* G_0 + \cdots = G_0 + G_0\Sigma^* G$$

(should be understood as matrix multiplication)

$$G(\omega) = \frac{G_0(\omega)}{1 - \Sigma^*(\omega) G_0(\omega)}$$

(Matrix inversion)

Quasi-particle equation

$$G(x,x';\omega) = G_0(x,x';\omega) + \int dx_1\, dx_2 G_0(x,x_1;\omega)\Sigma^*(x_1,x_2;\omega)G(x_2,x';\omega)$$

$$[\omega - \hat{h}_0(x)]G_0(x,x';\omega) = \delta(x-x')$$

$$[\omega - \hat{h}_0(x)]G(x,x';\omega) = \delta(x-x') + \int dx_2\, \Sigma^*(x,x_2;\omega)G(x_2,x',\omega)$$

Or

$$[\omega - \hat{h}_0(x)]G(x,x';\omega) - \int dx_1\, \Sigma^*(x,x_1;\omega)G(x_1,x',\omega) = \delta(x-x')$$

$$G_0(x,x';\omega) = \sum_n \frac{\phi_n(x)\phi_n^*(x')}{\omega - \epsilon_n}$$

Similarly $$G(x,x';\omega) = \sum_n \frac{\psi_n^L(x,\omega)\psi_n^R(x',\omega)}{\omega - \xi_n(\omega)}$$

Quasi-particle equation

$$[\omega - \hat{h}_0(x)]G(x,x';\omega) - \int dx_1\, \Sigma^*(x,x_1;\omega)G(x_1,x',\omega) = \delta(x-x')$$

$$G_0(x,x';\omega) = \sum_n \frac{\phi_n(x)\phi_n^*(x')}{\omega - \epsilon_n}, \qquad \hat{h}_0\phi_n(x) = \epsilon_n\phi_n(x)$$

$$G(x,x';\omega) = \sum_n \frac{\psi_n^R(\omega,x)\psi_n^L(\omega,x')}{\omega - \xi_n(\omega)} \qquad \left(\sum_n \psi_n^L(\omega,x)\psi_n^R(\omega,x') = \delta(x-x')\right)$$

$$\hat{h}_0\psi_n^R(\xi_n,x) + \int dx'\Sigma^*(x,x',\omega)\psi_n^R(\omega,x') = \xi_n(\omega)\psi_n^R(\omega,x)$$

Quasi-particle approximation: only one pole for a given *n*; ξ_n, ψ_n don't depend on ω ➡

$$\hat{h}_0\psi_n(x) + \int dx'\Sigma^*(x,x',\xi_n)\psi_n(x') = \xi_n\psi_n(x)$$

Comparison between the Kohn-Sham equation and quasi-particle equation

Let $\hat{h}_H = \hat{h}_0 + \hat{v}_{Hartree}(x) = -\frac{\nabla^2}{2} + \hat{v}_{ext}(x) + \hat{v}_{Hartree}(\mathbf{r})$

The Kohn-Sham equation:

$$\hat{h}_H \phi_n(x) + \hat{V}_{xc}(x)\phi_n(x) = \epsilon_n \phi_n(x)$$

Quasi-particle equation (not an Hermitian eigenvalue equation):

$$\hat{h}_H \psi_n(x) + \int dx' \Sigma^*_{xc}(x, x', \xi_n)\psi_n(x') = \xi_n \psi_n(x)$$

$$\Sigma^* = V_{Hartree} + \Sigma^*_{xc}$$

The self-energy is non-local, complex, and dynamical;

The effective Hamiltonian is non-Hermitian.

Perturbative calculation of the quasiparticle energy

Assuming: $\psi_n(x) \approx \phi_n(x)$

The quasiparticle energy:

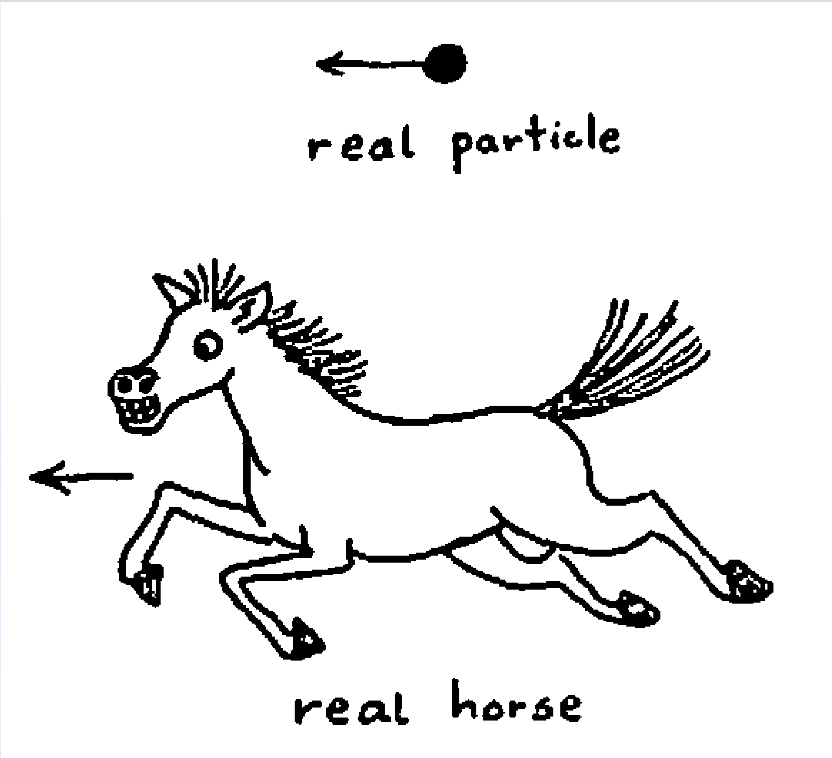
$$E_n = \mathrm{Re}[\xi_n] = \epsilon_n + \mathrm{Re}[\langle \phi_n \mid \Sigma^*_{xc}(\xi_n) - V_{xc} \mid \phi_n \rangle]$$
$$= \epsilon_n + Z_n \mathrm{Re}[\langle \phi_n \mid \Sigma^*_{xc}(\epsilon_n) - V_{xc} \mid \phi_n \rangle]$$

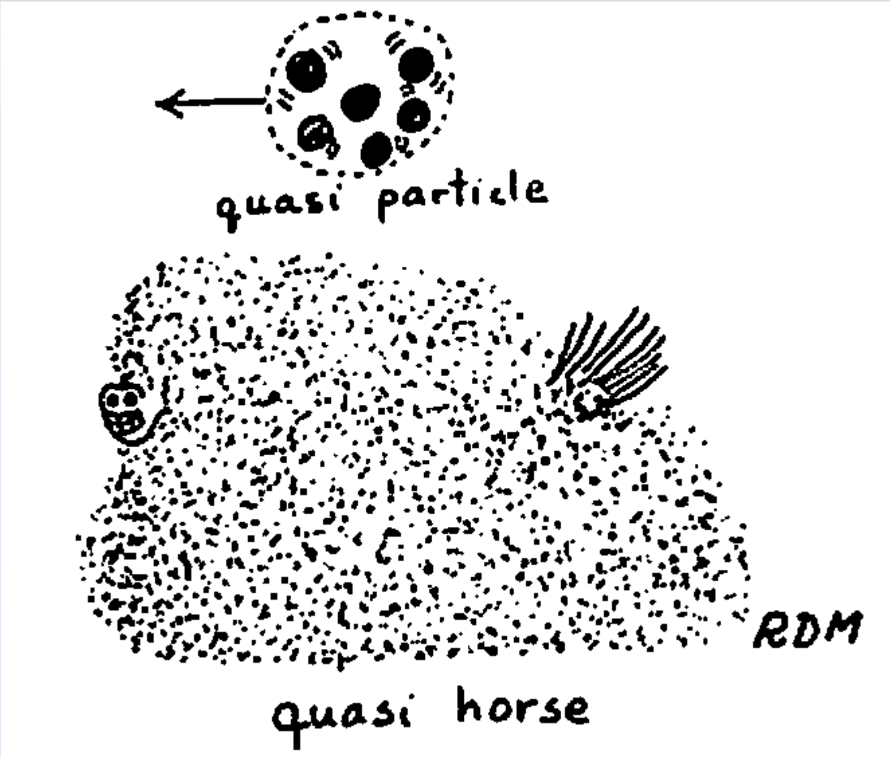
Quasiparticle weight

$$Z_n = \left(1 - \left[\frac{\partial \mathrm{Re} \langle \Sigma^*_{xc}(\omega) \rangle_n}{\partial \omega} \right]_{\omega = \epsilon_n} \right)^{-1}$$

The imaginary part of the self-energy measures the lifetime of the quasiparticle excitation!

Physical picture of quasiparticle





Real particle + “cloud” of other particle = quasi particle

Physical picture of quasiparticle

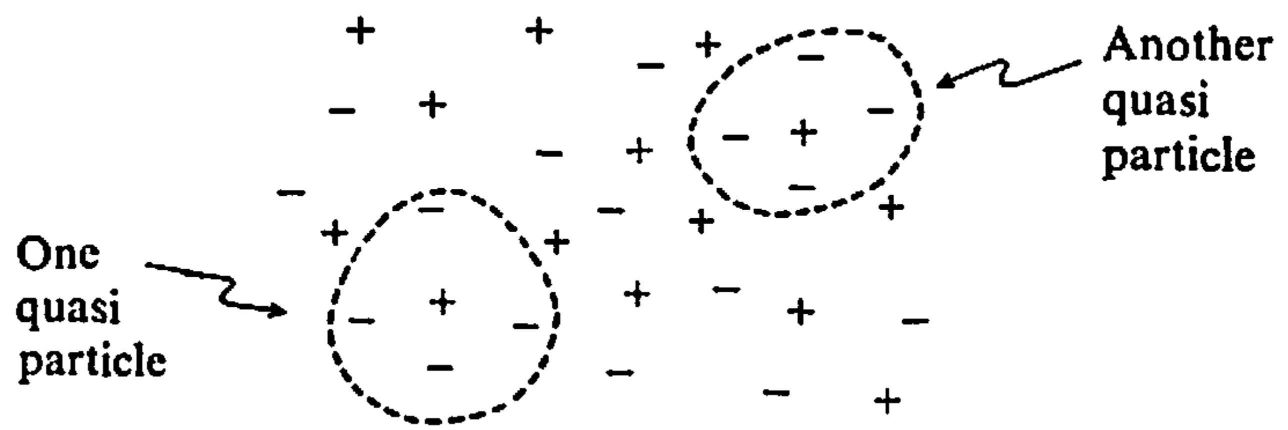
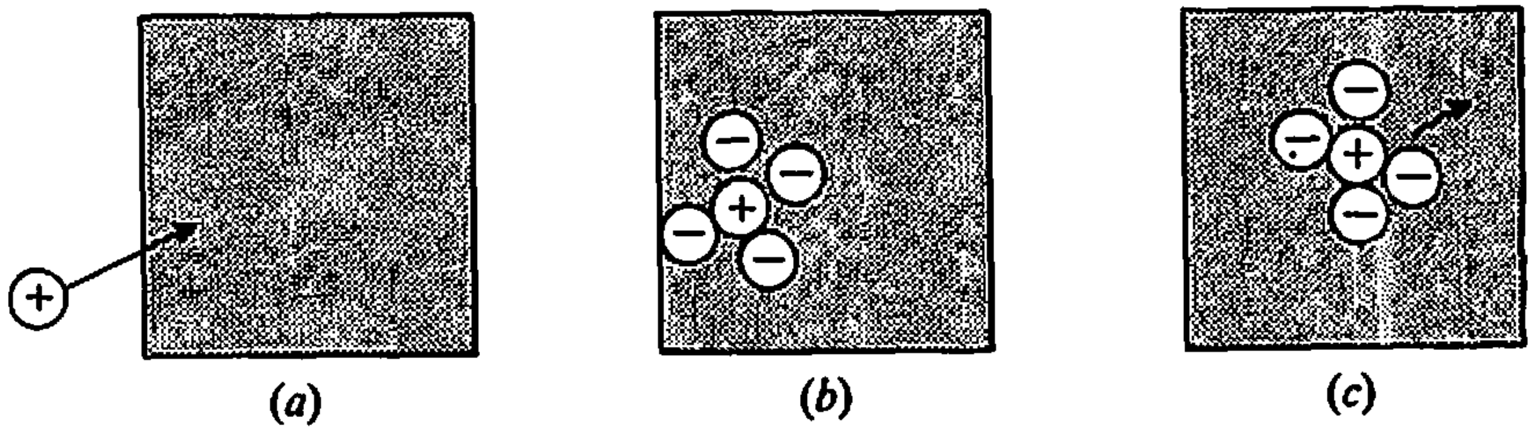


Fig. 0.5 *Quasi Particles in a Liquid of Positive and Negative Ions*



(a)Add a bare particle to the system; (b) Form a quasiparticle;
(c) Moving of the quasiparticle.

Reference

Richard D. Mattuck,

"A Guide to Feynman Diagrams in the Many-Body Problem"

Dover Publications, INC., New York, 1992