ELECTRONS WITHOUT OPERATORS

I. ONE ELECTRON

Feynamn path integrals.

II. MANY ELECTRONS

Functional integrals over Grassman fields.

I. ONE ELECTRON

CM: want path

$$x(t)\ ,\ p(t)$$

All we need is the hamiltonian *function*

$$H(p,x)$$

Can solve Hamilton's eqs.

$$\begin{cases} \frac{dx}{dt} & = & \frac{\partial H(p,x)}{\partial p} \\ \frac{dp}{dt} & = & -\frac{\partial H(p,x)}{\partial x} \end{cases}$$

or, equivalently, use the variational principle

$$\delta S[p,x] = 0$$

$$S[p,x] = \int_{t_i}^{t_f} dt \left\{ p\frac{dx}{dt} - H(p,x) \right\}$$

class. action

QM: want quantum-mechanical state

$$|\psi(t)>$$

can get it from the Hamiltonian *operator*

$$H(\widehat{p}, \widehat{x})$$

by solving Schrödinger's eq.

$$i\hbar\frac{\partial}{\partial t}|\psi(t)> = H(\widehat{p}, \widehat{x})|\psi(t)>$$

Looks very different.

May make it closer by writing QM in terms of $H(p, x)$.

Evolution of QM state:

$$i\hbar\frac{\partial}{\partial t}|\psi(t)>= H(\widehat{p},\widehat{x})|\psi(t)>\Rightarrow$$

$$\Rightarrow |\psi\left(t_f\right)\rangle = e^{-\frac{i}{\hbar}H(\widehat{p},\widehat{x})\left(t_f-t_i\right)}|\psi(t_i)\rangle$$

$$U\left(t_f-t_i\right) \equiv e^{-\frac{i}{\hbar}H(\widehat{p},\widehat{x})\left(t_f-t_i\right)}$$

time-evolution operator

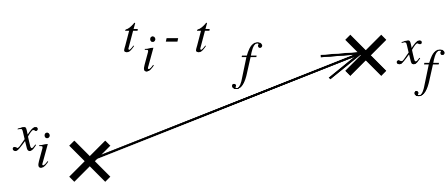
Evolution of wave function:

$$\langle x_f|\psi\left(t_f\right)\rangle = \int dx \langle x_f|U\left(t_f-t_i\right)|x\rangle\langle x|\psi(t_i)\rangle$$

$\Rightarrow$ if $|\psi(t_i)\rangle = |x_i\rangle$, then

$$\langle x_f|\psi\left(t_f\right)\rangle = \langle x_f|U\left(t_f-t_i\right)|x_i\rangle$$

Gives amplitude for



Want "formula" without $\widehat{p},\widehat{x}$

For any operator

$$\hat{O} = \int dpdx|p >< p|\hat{O}|x >< x| \qquad (1)$$

(from $\int dx|x >< x| = 1$, $\int dp|p >< p| = 1$).

If $H(\widehat{p},\widehat{x})$ normal-ordered (use $[\widehat{p},\widehat{x}] = i\hbar$) can relate $H(p,x)$ to $H(\widehat{p},\widehat{x})$:

$$\langle p|H(\widehat{p},\widehat{x})|x\rangle = \langle p|x\rangle H(p,x) \qquad (2)$$

$$\langle x|p\rangle = (2\pi\hbar)^{-1/2}\, e^{ipx/\hbar} \ \text{(plane w.)}$$

Using (1) and (2) can do

$$H(\widehat{p},\widehat{x}) \ \rightarrow \ H(p,x)$$

Split time-evolution:

$$\langle x_f | U\left(t_f - t_i\right) | x_i \rangle = \langle x_f | e^{-\frac{i}{\hbar} H(\widehat{p},\widehat{x})\delta t} \ldots e^{-\frac{i}{\hbar} H(\widehat{p},\widehat{x})\delta t} | x_i \rangle \qquad (3)$$

Each term linear in $H(\widehat{p}, \widehat{x})$

$$e^{-\frac{i}{\hbar} H(\widehat{p},\widehat{x})\delta t} \approx 1 - \frac{i}{\hbar} H(\widehat{p}, \widehat{x})\,\delta t$$

so can use previous formulae (1,2)

$$1 - \frac{i}{\hbar} H(\widehat{p}, \widehat{x})\,\delta t =$$

$$= \int dpdx\ |p >< p| \left(1 - \frac{i}{\hbar} H(\widehat{p}, \widehat{x})\,\delta t\right) |x >< x|$$

$$= \int dpdx\ |p >< p|x > \left(1 - \frac{i}{\hbar} H(p, x)\,\delta t\right) < x|$$

$$= \int dpdx\ |p >< p|x > e^{-\frac{i}{\hbar} H(p,x)\delta t} < x| \qquad (4)$$

Insert (4) in (3) - *no hats!*

But N.B. *many integrals*
(one $\int dp_k dx_k$ for each t_k)

The final formula:

$$\langle x_f | U\left(t_f - t_i\right) | x_i \rangle =$$

$$= \langle x_f | e^{-\frac{i}{\hbar}H(\widehat{p},\widehat{x})\delta t} ... e^{-\frac{i}{\hbar}H(\widehat{p},\widehat{x})\delta t} ... e^{-\frac{i}{\hbar}H(\widehat{p},\widehat{x})\delta t} | x_i \rangle =$$

$$= \int dp_{M-1} dx_{M-1} ... \int dp_k dx_k ... \int dp_0 dx_0$$

$$\langle x_f | p_{M-1} \rangle \langle p_{M-1} | x_{M-1} \rangle e^{-\frac{i}{\hbar}H\left(p_{M-1},x_{M-1}\right)\delta t} \langle x_{M-1} | ...$$

$$... | p_k \rangle \langle p_k | x_k \rangle e^{-\frac{i}{\hbar}H(p_k,x_k)\delta t} \langle x_k | ...$$

$$... | p_0 \rangle \langle p_0 | x_0 \rangle e^{-\frac{i}{\hbar}H(p_0,x_0)\delta t} \langle x_0 | x_i \rangle =$$

$$\left[\begin{array}{c} \langle p_k | x_k \rangle = (2\pi\hbar)^{-1/2}\, e^{-\frac{i}{\hbar}p_k x_k} \\ \langle x_{k+1} | p_k \rangle = (2\pi\hbar)^{-1/2}\, e^{\frac{i}{\hbar}p_k x_{k+1}} \\ \langle x_0 | x_i \rangle = \delta\left(x_0 - x_i\right) \end{array} \right]$$

$$= \int \prod_{k=0}^{M-1} dp_k \prod_{k=1}^{M-1} dx_k \frac{1}{2\pi\hbar} e^{\frac{i}{\hbar}\sum_{k=0}^{M-1}\left\{p_k\left(x_{k+1}-x_k\right)-\frac{i}{\hbar}H(p_k,x_k)\right.}$$

$$x_M \equiv x_f \;,\; x_0 \equiv x_i \quad \text{(boundary conditions)}$$

''Elegant'' notation:

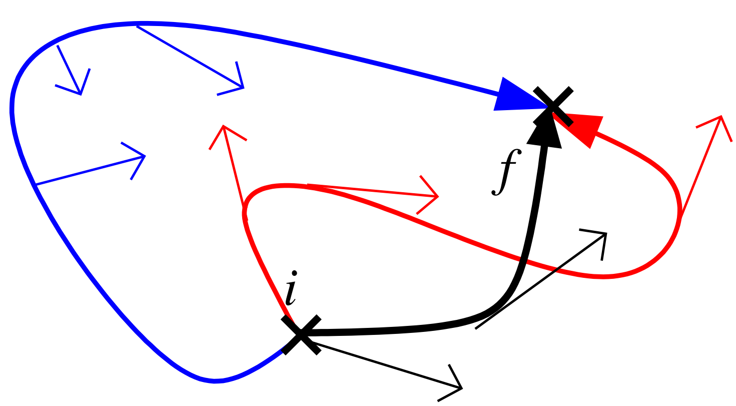
$$\langle x_f | U\left(t_f - t_i\right) | x_i \rangle \equiv \int_{x(t_i)=x_i, x(t_f)=x_f} Dx Dp \; e^{\frac{i}{\hbar} S[p,x]}$$

$$S[p,x] = \int_{t_i}^{t_f} dt \left\{ p(t)\,\dot{x}(t) - H\left(p(t), x(t)\right) \right\}$$

classical action

Integrate all paths:

- **classical** and non-classical
- $p(t) \neq m\dot{x}(t)$



Achieved

$$H(\hat{p}, \hat{x}) \;\rightarrow\; H(p, x)$$

The price

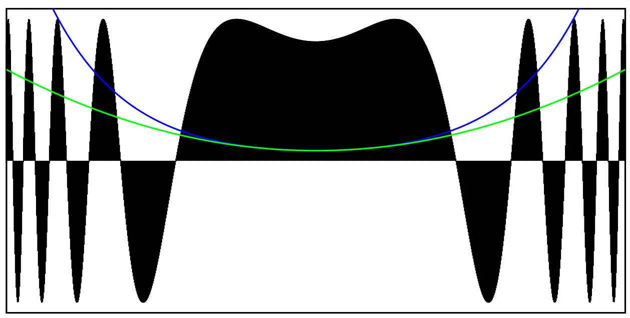
differential equation $\rightarrow$ functional integral

Usually new problem more difficult (H atom).

But also new approximations (e.g. MC).

Stationary phase approximation:

$$\int du e^{if(u)} \, , \; \delta f \left(u = u_0 \right) = 0$$



$$\text{expand}: \; f(u) \approx f(u_0) + \frac{1}{2} f''(u_0) (u - u_0)^2$$

$$\int du e^{if(u)} \approx e^{if(u_0)} \int du e^{i\frac{f''(u_0)}{2} u^2}$$

$$[\text{Fresnel integral}] = e^{if(u_0)} \left(\sqrt{\frac{2\pi}{f''(u_0)}} e^{i\pi/4} \right)$$

$$(\text{condition}: \; f(u + \Delta u) - f(u) \gg 2\pi)$$

More than one stationary point $u_0, u_1, ...$:

$$\int du e^{if(u)} \approx e^{if(u_0)} (...) + e^{if(u_1)} (...) + ...$$

$$I \equiv \int_{-\infty}^{\infty} du e^{iau^2} = \frac{1}{\sqrt{a}} \int_{-\infty}^{\infty} du e^{iu^2}$$

$$= \frac{2}{\sqrt{a}} \left\{ \int_0^{\infty} du \cos\left(u^2\right) + i \int_0^{\infty} du \sin\left(u^2\right) \right\}$$

Fresnel integrals:

$$S(v) = \sqrt{\frac{2}{\pi}} \int_0^v \sin\left(u^2\right) du$$

$$C(v) = \sqrt{\frac{2}{\pi}} \int_0^v \cos\left(u^2\right) du$$

Thus

$$I = \sqrt{\frac{2\pi}{a}} \underbrace{\left\{ \underbrace{C(\infty)}_{1/2} + i \underbrace{S(\infty)}_{1/2} \right\}}_{e^{i\pi/4}/\sqrt{2}} = \sqrt{\frac{\pi}{a}} e^{i\pi/4}$$

But

$$\frac{1}{\hbar}S\left[p+\Delta p,x+\Delta x\right]-\frac{1}{\hbar}S\left[p,x\right]\gg 2\pi$$

when

$$S\left[p,x\right]\gg\hbar$$

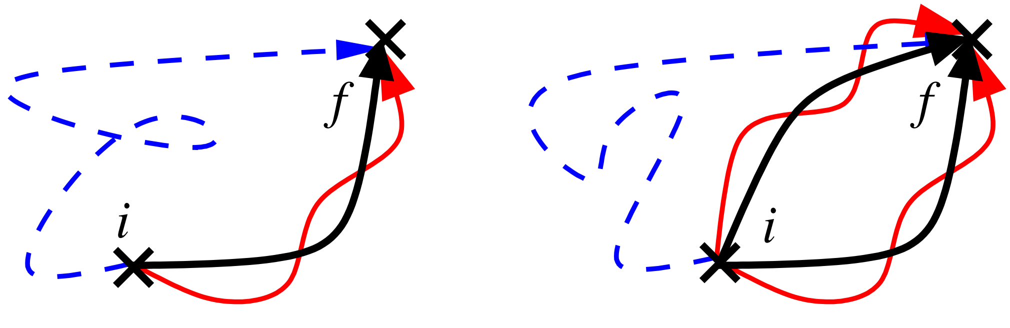
(semiclassical).

Saddle point:

$$\delta S\left[p,x\right]=0$$

(Hamilton's variational principle of CM)

$$\langle x_f|U\left(t_f-t_i\right)|x_i\rangle\equiv\sum_{\text{class. paths}}e^{\frac{i}{\hbar}S[p_{cl},x_{cl}]}(\ldots)$$



classical + fluctuations (order$-n$) + interference

II. MANY ELECTRONS - $H\left(\widehat{p}_1, ..., \widehat{p}_N, \widehat{x}_1, ..., \widehat{x}_N\right)$

Statistical mechanics:

$$Z = \mathrm{tr}\left\{e^{-\beta H(\widehat{p},\widehat{x})}\right\}$$

$$\left[\mathrm{tr}\left\{\hat{O}\right\} = \int dx \langle x|\hat{O}|x\rangle\right] = \int dx \langle x|U\left(-i\hbar\beta\right)|x\rangle$$

Can use Feynman path integral for

$$\langle x_f|U\left(t_f - t_i\right)|x_i\rangle$$

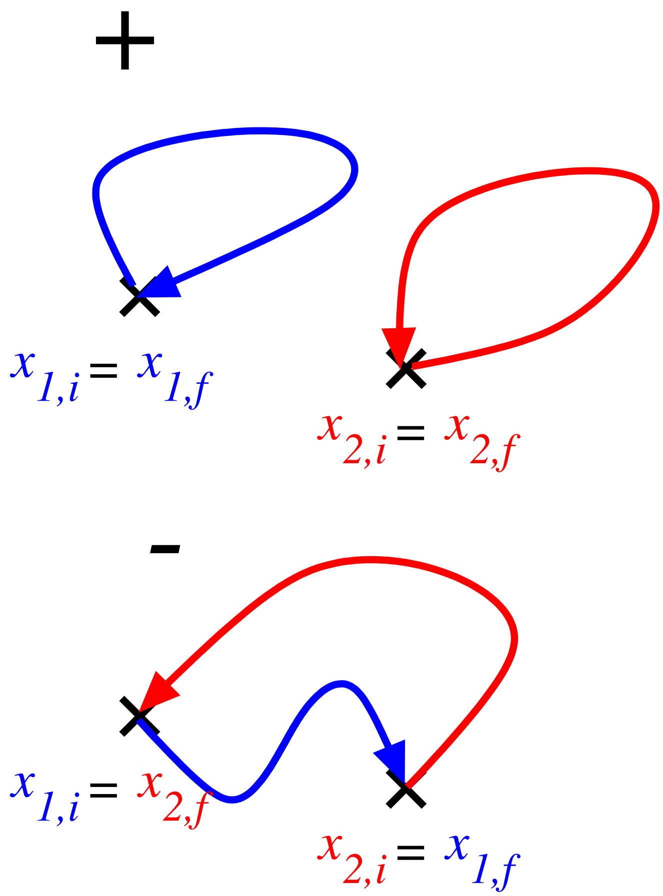
- Imaginary time $\tau = (i/\hbar)\, t$
- All periodic orbits: $\tau_f - \tau_i = \beta$, $x\left(\tau_f\right) = x\left(\tau_i\right)$

BUT a complication for many particles

$$\psi\left(...x_{i,f}...x_{j,f}..., t_f\right) = -\psi\left(...x_{j,f}...x_{i,f}..., t_f\right)$$

Not included in Schrödinger Equation
$\Rightarrow$ need to "complete" our formula

Need to give each path a sign:



Complicated!

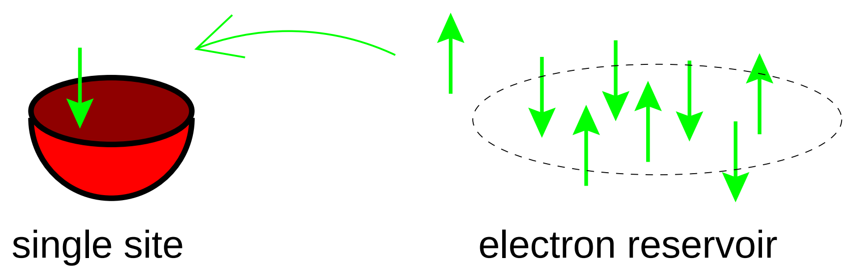
This problem not exclusive to path integrals.

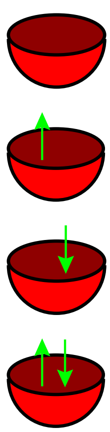
We want to have the symmetry inside $\widehat{H}$.

Second quantization:

Fock space ***F***
- a subset of ***H***
- all the states with the right symmetry

<u>e.g.</u> one-site Hubbard model





$|0\rangle$

$|\uparrow\rangle$

$|\downarrow\rangle$

$|\uparrow\downarrow\rangle = (|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle)/\sqrt{2}$

_ $\neq (|\uparrow\rangle|\downarrow\rangle + |\downarrow\rangle|\uparrow\rangle)/\sqrt{2}$ (e.g.)

_ ***F*** has only 4 states ***(H*** has ∞)

Operators in Fock space:

$$\widehat{c}_r^{+}|...n_r...\rangle \equiv (1-n_r)\,|...n_r+1...\rangle \quad \text{(creation)}$$
$$\widehat{c}_r|...n_r...\rangle \equiv n_r|...n_r-1...\rangle \quad \text{(destruction)}$$

($\Rightarrow$ density given by $\widehat{c}_r^{+}\widehat{c}_r|...n_r...\rangle = n_r|...n_r...\rangle$)

N.B. the labels are not particles, but 1-particle states.

Using $\widehat{c}^{+}$, $\widehat{c}$

1. Can go all over ***F***
   $\Rightarrow$ can write $H\left(\widehat{c}^{+},\widehat{c}\right)$

   e.g.

   $$H\left(\widehat{c}^{+},\widehat{c}\right) = (\varepsilon_0-\mu)\left(\widehat{c}_\uparrow^{+}\widehat{c}_\uparrow + \widehat{c}_\downarrow^{+}\widehat{c}_\downarrow\right) + u\widehat{c}_\uparrow^{+}\widehat{c}_\uparrow\widehat{c}_\downarrow^{+}\widehat{c}_\downarrow$$

2. We stay in ***F***
   $\Rightarrow H\left(\widehat{c}^{+},\widehat{c}\right)$ *contains the symmetry!*

N.B. we have defined $\hat{c}$ by how it acts on the Slater determinants such as $|\uparrow\downarrow\rangle$. How does it act on the simple products of one-particles states, such as $|\uparrow\rangle|\downarrow\rangle$, that the Slater determinants are defined in terms of? We can deduce it from the definition. For example,

$$\hat{c}_\uparrow|\uparrow\downarrow\rangle = \hat{c}_\uparrow\left(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle\right)/\sqrt{2} \equiv |\downarrow\rangle$$

$$\Rightarrow \hat{c}_\uparrow|\uparrow\rangle|\downarrow\rangle = |\downarrow\rangle/\sqrt{2}\,,\; \hat{c}_\uparrow|\downarrow\rangle|\uparrow\rangle = -|\downarrow\rangle/\sqrt{2}$$

This is important because coherent states are defined in terms of these states (not of states of the Fock space) -we need, it, for example, to prove that they are really coherent. We also need that $|0\rangle|r\rangle = |r\rangle$ (i.e. $|0\rangle$ is the neutral element, not the null one, which is 0).

Commutation rules:

$$\hat{c}_i^{+}\hat{c}_j + \hat{c}_j^{+}\hat{c}_i = \delta_{ij}$$

	$\|n\rangle = \|0\rangle$	$\|n\rangle = \|1\rangle$
$\hat{c}^{+}\hat{c}\|n\rangle$	0	$\|1\rangle$
$\hat{c}\hat{c}^{+}\|n\rangle$	$\|0\rangle$	0
$\left(\hat{c}^{+}\hat{c} + \hat{c}\hat{c}^{+}\right)\|n\rangle$	$\|0\rangle$	$\|1\rangle$

Similarly

$$\hat{c}_i\hat{c}_j + \hat{c}_j\hat{c}_i = \delta_{ij}$$

$$\hat{c}_i^{+}\hat{c}_j^{+} + \hat{c}_j^{+}\hat{c}_i^{+} = \delta_{ij}$$

In 1st quantization we had

$$Z = \mathrm{tr}\left\{ \mathrm{e}^{-\beta H(\hat{p},\hat{x})} \right\}$$

Got rid of operators using

$$\langle p|\hat{p} = \langle p|p \quad , \quad \hat{x}|x\rangle = x|x\rangle$$

$$\Rightarrow \langle p|H\left(\hat{p},\hat{x}\right)|x\rangle = \langle p|x\rangle H\left(p,x\right)$$

Now 2nd quantisation:

$$Z = \mathrm{tr}\left\{ \mathrm{e}^{-\beta H\left(\hat{c}^{+},\hat{c}\right)} \right\}$$

Want "coherent states"

$$\langle\overline{c}|\hat{c}^{+} = \langle\overline{c}|\overline{c} \quad , \quad \hat{c}|c\rangle = c|c\rangle$$

$$\Rightarrow \langle\overline{c}|H\left(\hat{c}^{+},\hat{c}\right)|c\rangle = \langle\overline{c}|c\rangle H\left(p,x\right)$$

But writing

$$|c\rangle = \langle 0|c\rangle|0\rangle + \langle 1|c\rangle|1\rangle$$

we have

$$\hat{c}|c\rangle = c|c\rangle \Rightarrow \langle 0|c\rangle = \langle 1|c\rangle = 0$$

¡coherent states do not exist!

Let us *enlarge* ***F***:

1. Define *Grassman numbers*:

$$a, b \text{ Grassman } \Leftrightarrow ab = -ba$$

(N.B. $a^2 = 0$ and $f(a) = f(0) + f'(0)\, a$)

2. Allow for new type of states:

$$|\psi\rangle = \sum_r \langle r|\psi\rangle |r\rangle$$

$\langle 0|\psi\rangle, \langle 1|\psi\rangle$ contain Grassman numbers

The coherent states are

$$|c\rangle \equiv |c_1 c_2 ...\rangle \;=\; \prod_r \left(|0\rangle + c_r |r\rangle\right)$$
$$\langle \bar{c}| \equiv \langle \bar{c}_1 \bar{c}_2 ...| \;=\; \prod_r \left(\langle 0| + \bar{c}_r \langle r|\right)$$

e.g.

$$|c\rangle \equiv |c_\uparrow c_\downarrow\rangle \;=\; \Big(|0\rangle + c_\uparrow |\uparrow\rangle\Big)\Big(|0\rangle + c_\downarrow |\downarrow\rangle\Big)$$
$$\langle \bar{c}| \equiv \langle \bar{c}_\uparrow \bar{c}_\downarrow| \;=\; \Big(\langle 0| + \bar{c}_\uparrow \langle \uparrow|\Big)\Big(\langle 0| + \bar{c}_\downarrow \langle \downarrow|\Big)$$

Proof that they really are coherent states:

$$
\begin{aligned}
\hat{c}_\uparrow|c_\uparrow c_\downarrow> &= \hat{c}_\uparrow\left(|0\rangle + c_\uparrow|\uparrow\rangle\right)\left(|0\rangle + c_\downarrow|\downarrow\rangle\right)\\
&= \hat{c}_\uparrow(|0\rangle|0\rangle + c_\uparrow|\uparrow\rangle|0\rangle + c_\downarrow|0\rangle|\downarrow\rangle\\
&\quad +c_\uparrow c_\downarrow|\uparrow\rangle|\downarrow\rangle)\\
&= \hat{c}_\uparrow\underbrace{|0\rangle|0\rangle}_{|0\rangle} + c_\uparrow\hat{c}_\uparrow\underbrace{|\uparrow\rangle|0\rangle}_{|\uparrow\rangle} + c_\downarrow\hat{c}_\uparrow\underbrace{|0\rangle|\downarrow\rangle}_{|\downarrow\rangle}\\
&\quad +c_\uparrow c_\downarrow\hat{c}_\uparrow|\uparrow\rangle|\downarrow\rangle\\
&= 0 + c_\uparrow|0\rangle + c_\downarrow 0 + c_\uparrow c_\downarrow\underbrace{|0\rangle|\downarrow\rangle}_{|\downarrow\rangle}\\
&= c_\uparrow(\underbrace{|0\rangle}_{|0\rangle|0\rangle} + c_\downarrow\underbrace{|\downarrow\rangle}_{|0\rangle|\downarrow\rangle})\\
\left[c_\uparrow c_\uparrow = 0\right] &= c_\uparrow(|0\rangle|0\rangle + c_\uparrow|\uparrow\rangle|0\rangle + c_\downarrow|0\rangle|\downarrow\rangle\\
&\quad +c_\uparrow c_\downarrow|\uparrow\rangle|\downarrow\rangle) = c_\uparrow|c_\uparrow c_\downarrow> \quad \text{Q.E.D.}
\end{aligned}
$$

Recall

$$Z = \text{tr}\left\{e^{-\beta H(\hat{p},\hat{x})}\right\} = \int dx \langle x|e^{-\beta H(\hat{p},\hat{x})}|x\rangle$$

$$\int dx dp \langle x|p\rangle |x\rangle\langle p| = 1$$

Need to define "$\int$" over Grassman numbers:

$$\int dadb\ ba \equiv 1$$

$$\int dadb\ ab \equiv -1$$

$$\int dadb \text{ (anything else)} \equiv 0$$

Get the *analgoues*

$$Z = \text{tr}\left\{e^{-\beta H\left(\hat{c}^{+},\hat{c}\right)}\right\} = \int \prod d\bar{c}dc\, e^{-\sum \bar{c}c}\langle -\bar{c}|e^{-\beta H(\bar{c},c)}|c\rangle$$

$$\int \prod d\bar{c}dce^{-\sum \bar{c}c}|c\rangle\langle \bar{c}| = 1$$

The *result* is

$$Z = \int_{c(\beta)=-c(0),\bar{c}(\beta)=-\bar{c}(0)} D\bar{c}Dc\, e^{-S[\bar{c},c]}$$

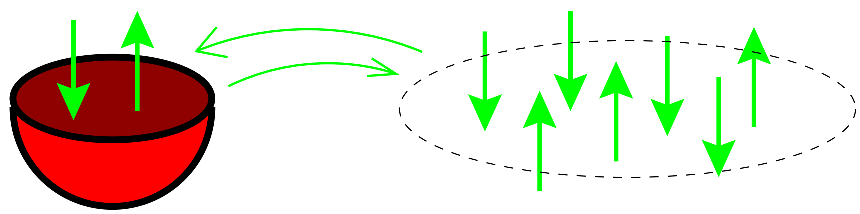
$$D\bar{c}Dc \equiv \prod_{\tau=\delta\tau}^{\beta} \prod_{r} d\bar{c}_r(\tau)\, dc_r(\tau)$$

$$\begin{aligned} S[\bar{c},c] \;&\equiv\; \delta\tau \sum_{\tau=\delta\tau}^{\beta} \{ \sum_r \bar{c}_r(\tau) \frac{c_r(\tau) - c_r(\tau-\delta\tau)}{\delta\tau} \\ &\qquad + H(\bar{c}(\tau), c(\tau-\delta\tau)) \} \\ &\equiv\; \int_0^{\beta} d\tau \left\{ \sum \bar{c}(\tau)\, \partial_\tau c(\tau) + H(\bar{c}(\tau), c(\tau)) \right\} \end{aligned}$$

(N.B. *anti*periodic boundary conditions)

(N.B. discrete definition rules)

EXAMPLE: one site, non-interacting e^-



$$H\left(\hat{c}^+, \hat{c}\right) = (\varepsilon_0 - \mu)\left(\hat{c}_\uparrow^+ \hat{c}_\uparrow + \hat{c}_\downarrow^+ \hat{c}_\downarrow\right)$$

Action:

$$\begin{aligned} S[\bar{c}, c] &= \int_0^\beta d\tau \left\{ \sum_\sigma \bar{c}_\sigma(\tau)\, \partial_\tau c_\sigma(\tau) + \varepsilon \sum_\sigma \bar{c}_\sigma(\tau)\, c_\sigma(\tau) \right\} \\ &= \sum_\sigma \int_0^\beta d\tau \bar{c}_\sigma(\tau) (\partial_\tau + \varepsilon)\, c_\sigma(\tau) \end{aligned}$$

$$= \sum_{l=1}^{M} \sum_\sigma \left\{ \bar{c}_\sigma(\tau_l) \left[c_\sigma(\tau_l) - c_\sigma(\tau_{l-1}) \right] + \frac{\beta}{M} \varepsilon \bar{c}_\sigma(\tau_l)\, c_\sigma(\tau_{l-1}) \right\}$$

$$= \sum_\sigma \sum_{i,j=1}^{M} \bar{c}_\sigma(\tau_i)\, A_{ij} c_\sigma\left(\tau_j\right)$$

$$A = \begin{pmatrix} 1 & & & & 1 - \frac{\beta\varepsilon}{M} \\ -1 + \frac{\beta\varepsilon}{M} & 1 & & & \\ & -1 + \frac{\beta\varepsilon}{M} & 1 & & \\ & & \ddots & \ddots & \\ & & & -1 + \frac{\beta\varepsilon}{M} & 1 \end{pmatrix}$$

Partition function:

$$Z = \int \prod_\sigma d\bar{c}_\sigma dc_\sigma e^{-\sum_\sigma \bar{c}_\sigma A c_\sigma}$$
$$= \prod_\sigma \int d\bar{c}_\sigma dc_\sigma e^{-\bar{c}_\sigma A c_\sigma} = \left(\int d\bar{c} dc e^{-\bar{c}Ac}\right)^2$$

Use *Gaussian integral*:

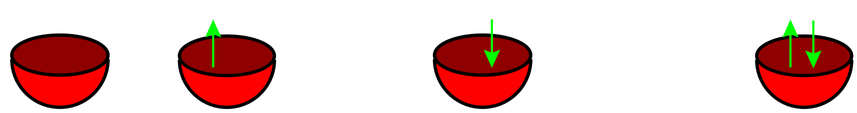
$$\int \prod_i d\bar{c}_i dc_i \, e^{-\sum_{ij} \bar{c}_i A_{ij} c_j} = ||A||$$

(Proof of the simplest case: $\int d\bar{c}dc\, e^{-\bar{c}Ac} = \int d\bar{c}dc\, (1 - \bar{c}Ac) = \int d\bar{c}dc\, 1 - A \int d\bar{c}dc\; \bar{c}c = A$)

$$||A|| = ||\partial_\tau + \varepsilon|| = 1 + (1 - \beta\varepsilon/M)^M = 1 + e^{-\beta\varepsilon}$$

$$Z = \left(1 + e^{-\beta\varepsilon}\right)^2$$

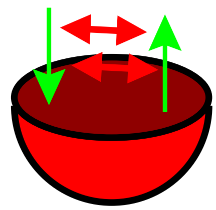
$$= 1 + e^{-\beta(\varepsilon_0 - \mu)} + e^{-\beta(\varepsilon_0 - \mu)} + e^{-\beta(2\varepsilon_0 - \mu 2)}$$



(as expected)

Proofs in

- 6/7/00 (non-interacting one-site)
- 2/7/00 (Gaussian integral, general case)

If we turn on an interaction 

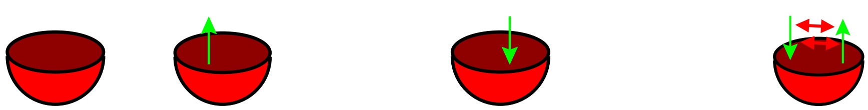
$$H\left(\hat{c}^{+},\hat{c}\right)=(\varepsilon_0-\mu)\left(\hat{c}^{+}_{\uparrow}\hat{c}_{\uparrow}+\hat{c}^{+}_{\downarrow}\hat{c}_{\downarrow}\right)+u\hat{c}^{+}_{\uparrow}\hat{c}_{\uparrow}\hat{c}^{+}_{\downarrow}\hat{c}_{\downarrow}$$

there is a quartic term $\Rightarrow$ can't use Gaussian.

However in this system with few (2) states the integral can still be done.

We obtain

$$Z=1+e^{-\beta(\varepsilon_0-\mu)}+e^{-\beta(\varepsilon_0-\mu)}+e^{-\beta[2(\varepsilon_0-\mu)+u]}$$



(correct!)

Proofs in 7/7/00

In general we can't solve problems with an interaction term exactly.

Need approximation schemes.

For Grassman integrals, we don't know any.

Trick: turn them into ordinary integrals using the *Hubbard-Stratonovich transformation*:

$$e^{b^2} = \frac{1}{\sqrt{\pi}} \int dx\, e^{-x^2+2bx} \quad \left(\text{from } \int dx\, e^{-x^2} = \sqrt{\pi}\right)$$

$$e^{\bar{b}b} = \frac{1}{2\pi i} \int dz^* \wedge dz\, e^{-z^* z + z^* b + z\bar{b}}$$

$$\left(\text{from } \int dz^* \wedge dz\, e^{-z^* z} = 2\pi i\right)$$

- $e^{b^2} = \dots \to$ 13/7/00, 21/7/00

- $e^{\bar{b}b} = \dots \to$ 9/10/00a

New (bosonic) fields have physical interpretation.

<u>e.g.</u> one-site with interaction

$$Z = \int D\bar{c}Dc\, e^{-\int_0^\beta \{\sum_\sigma \bar{c}_\sigma(\partial_\tau + \varepsilon)c_\sigma + u\bar{c}_\uparrow c_\uparrow \bar{c}_\downarrow c_\downarrow\}}$$

$$u\bar{c}_\uparrow c_\uparrow \bar{c}_\downarrow c_\downarrow = \frac{u}{2}\left(\bar{c}_\uparrow c_\uparrow + \bar{c}_\downarrow c_\downarrow\right)^2 \Rightarrow$$

$$\Rightarrow Z = \int D\varphi \int D\bar{c}Dc\, e^{-\int_0^\beta d\tau \left\{\frac{\varphi^2}{2} + \sum_\sigma \bar{c}_\sigma\left(\partial_\tau + \varepsilon + iu^{1/2}\varphi\right)c_\sigma\right\}}$$

("electrostatic" potential - e^--photons coupling)

$$u\bar{c}_\uparrow c_\uparrow \bar{c}_\downarrow c_\downarrow = u\bar{c}_\uparrow \bar{c}_\downarrow c_\downarrow c_\uparrow \Rightarrow$$

$$\Rightarrow Z = \int D\bar{\Delta} \wedge D\Delta \int D\bar{c}Dc$$

$$e^{-\int_0^\beta d\tau \left\{\frac{-|\Delta|^2}{u} + \sum_\sigma \bar{c}_\sigma(\partial_\tau + \varepsilon)c_\sigma - \bar{\Delta}c_\downarrow c_\uparrow - \Delta\bar{c}_\uparrow \bar{c}_\downarrow\right\}}$$

(pairing field - hybridized Bose-Fermi system)

Density - 13/7/00

Pairs - 9/10/00b

Fermionic system non-interacting
$\Rightarrow$ can do integrals (Gaussians).

<u>e.g.</u>

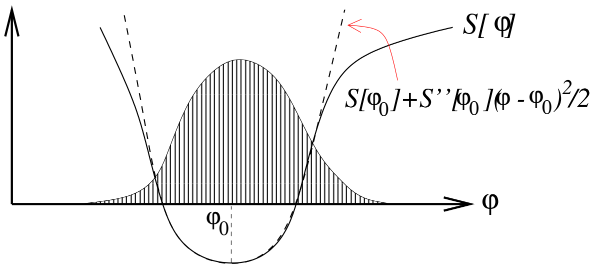
$$
\begin{aligned}
Z &= \int D\varphi \int D\bar{c}Dc\, e^{-\int_0^\beta d\tau \left\{\frac{\varphi^2}{2} + \sum_\sigma \bar{c}_\sigma \left(\partial_\tau + \varepsilon + iu^{1/2}\varphi\right) c_\sigma\right\}} \\
&= \int D\varphi\, e^{-\int_0^\beta d\tau \frac{\varphi^2}{2}} \int D\bar{c}Dc\, e^{-\int_0^\beta d\tau \sum_\sigma \bar{c}_\sigma \left(\partial_\tau + \varepsilon + iu^{1/2}\varphi\right)} \\
&= \int D\varphi\, e^{-S[\varphi]},\ S[\varphi] \equiv \int_0^\beta d\tau\, \frac{\varphi^2}{2} - \ln Z_f[\varphi]
\end{aligned}
$$

Solving the fermionic problem

$$
S[\varphi] = \int_0^\beta d\tau\, \frac{\varphi^2}{2} - 2\ln ||\partial_\tau + \varepsilon + iu^{1/2}\varphi||
$$

We are left with ordinary (difficult) integrals.

Saddle-point approximation:



$$\text{expand :}\quad S[\varphi] \approx S[\varphi_0] + \frac{1}{2} S''[\varphi_0](\varphi - \varphi_0)^2$$

$$\text{around } \delta S[\varphi] = 0$$

$$\int d\varphi e^{-S[\varphi]} \approx e^{-S[\varphi_0]} \int d\varphi e^{-\frac{1}{2}S''[\varphi_0]x^2}$$

$$\text{[Gaussian integral]} = e^{-S[x_0]}\sqrt{2\pi / S''[\varphi_0]}$$

Lowest order gives mean field:

$$\delta S[\varphi] = 0 \;\Rightarrow\; \delta\left(\int_0^\beta d\tau \frac{\varphi^2}{2} - \ln Z_f[\varphi]\right) = 0$$

$$\Rightarrow\; \varphi = u \left\langle \sum_\sigma \hat{c}_\sigma^+ \hat{c}_\sigma \right\rangle_f$$

$$\delta S[\bar{\Delta}, \Delta] = 0 \Rightarrow \Delta = u \left\langle \hat{c}_\uparrow \hat{c}_\downarrow \right\rangle_{BCS}$$

Higher-order $\Rightarrow$ fluctuations. N.B. no $1/\hbar$

BIBLIOGRAPHY

- Nagaosa - nice introduction

- Negele & Orland - drier but more useful

- Kleinert - this guy believes in Feynman path integrals (lots about this left unsaid!)