Second quantisation

Creation & annihilation operators

$$a_i^\dagger |\dots n_i \dots\rangle = \sqrt{n_i+1}\, |\dots n_i+1 \dots\rangle$$

$$a_i |\dots n_i \dots\rangle = \sqrt{n_i}\, |\dots n_i-1 \dots\rangle$$

Hamiltonian for system with discrete sites:

$$\hat{H}_{\text{mult}} = \sum_{ij} H(i,j)\, a_i^\dagger a_j + \frac{1}{2} \sum_{ij} U^{\text{int}}(i,j)\, a_i^\dagger a_j^\dagger a_j a_i$$

Continuous case

$i \to \underline{r}, \quad j \to \underline{r}'$

$a_i^+ \to a^+(\underline{r}), \quad a_i \to a(\underline{r}), \qquad [a(\underline{r}), a^+(\underline{r}')] = \delta(\underline{r}-\underline{r}')$

Hamiltonian

$$\hat{H} = \int d^n r \; a^+(\underline{r})\left(-\frac{\hbar^2}{2m}\nabla^2 + U(\underline{r})\right) a(\underline{r})$$

$$+ \frac{1}{2}\int d^n r \int d^n r' \; U^{int}(\underline{r},\underline{r}')\, a^+(\underline{r})\, a^+(\underline{r}')\, a(\underline{r}')\, a(\underline{r})$$

Single particle term looks similar to exp. value

$$\int d^n r \; \psi^*(\underline{r})\left(-\frac{\hbar^2}{2m}\nabla^2 + U(\underline{r})\right)\psi(\underline{r})$$

as if we replaced wavef. by operator (second quantisation)

4.6 Fermions

can't have two fermions in the same state

$$(a_i^+)^2 = 0$$

with anticommutator $[A,B]_+ = AB + BA$

$$[a_i^+, a_i^+]_+ = a_i^+ a_i^+ + a_i^+ a_i^+ = 0$$

demand

$$[a_i^+, a_j^+]_+ = [a_i, a_j]_+ = 0$$

$$[a_i, a_j^+]_+ = \delta_{ij}$$

This is satisfied for

$$a_i^\dagger |\ldots n_i = 0 \ldots\rangle = (-1)^{\sum_{k=1}^{i-1} n_k} |\ldots n_i = 1 \ldots\rangle \qquad (1)$$

$$a_i^\dagger |\ldots n_i = 1 \ldots\rangle = 0 \qquad (2)$$

$$a_i |\ldots n_i = 0 \ldots\rangle = 0 \qquad (3)$$

$$a_i |\ldots n_i = 1 \ldots\rangle = (-1)^{\sum_{k=1}^{i-1} n_k} |\ldots n_i = 0 \ldots\rangle \qquad (4)$$

Motivation:

- (1), (4) up to sign ✓
- (2), (3) as n_i can't be 2 or -1
- without signs

$$a_1^\dagger\, a_2^\dagger\, |0,0\rangle = a_1^\dagger\, |0,1\rangle = |1,1\rangle$$

$$a_2^\dagger\, a_1^\dagger\, |0,0\rangle = a_2^\dagger\, |1,0\rangle = |1,1\rangle \qquad ↯$$

with signs

$$a_1^\dagger\, a_2^\dagger\, |0,0\rangle = a_1^\dagger\, |0,1\rangle = |1,1\rangle$$

$$a_2^\dagger\, a_1^\dagger\, |0,0\rangle = a_2^\dagger\, |1,0\rangle = -\,|1,1\rangle \qquad ☺$$

- more generally

$$a_i^\dagger \, a_j^\dagger \, |\ldots n_i=0 \ldots n_j=0\ldots\rangle$$

$$= a_i^\dagger \, (-1)^{\sum_{k=1}^{j-1} n_k} \, |\ldots n_i=0 \ldots n_j=1\ldots\rangle$$

$$= (-1)^{\sum_{k=1}^{i-1} n_k} (-1)^{\sum_{k=1}^{j-1} n_k} |\ldots n_i=1 \ldots n_j=1\ldots\rangle$$

$$a_j^\dagger \, a_i^\dagger \, |\ldots n_i=0 \ldots n_j=0\ldots\rangle$$

$$= a_j^\dagger \, (-1)^{\sum_{k=1}^{i-1} n_k} \, |\ldots n_i=1 \ldots n_j=0\ldots\rangle$$

$$= (-1)^{\sum_{k=1}^{j-1} n_k + 1} (-1)^{\sum_{k=1}^{i-1} n_k} |\ldots n_i=1 \ldots n_j=1\ldots\rangle$$

- full derivation on problem sheet 6

5 Path integrals in second quantisation

5.1 Bosons

consider trace, first in single particle QM

$$\mathrm{tr}\, e^{-\frac{i}{\hbar}\hat{H}t} = \int d^n r \underbrace{\langle \underline{r} | e^{-\frac{i}{\hbar}\hat{H}t} | \underline{r} \rangle}_{K(\underline{r},\underline{r},t)}$$

Motivation:

- Stat Mech
  $\mathrm{tr}\, e^{-\beta\hat{H}}$ accessible through $\frac{i}{\hbar}t \to \beta$
- Quantum chaos
  level density $\sum_j \delta(E-E_j)$ accessible from propagator through operations that involve a trace

Hamiltonian mechanics path integral

$$\langle \underline{r}_f | e^{-\frac{i}{\hbar}\hat{H}t} | \underline{r}_0 \rangle = \int\limits_{\substack{\underline{r}(0)=\underline{r}_0 \\ \underline{r}(t)=\underline{r}_f}} \mathcal{D}[\underline{r}]\,\mathcal{D}[\underline{p}]\, \exp\left(\frac{i}{\hbar}\int_0^t [\underline{p}(t')\cdot\dot{\underline{r}}(t') - H(\underline{r}(t'),\underline{p}(t'))]\,dt'\right)$$

where $\int \mathcal{D}[\underline{r}]\,\mathcal{D}[\underline{p}]\ldots = \lim\limits_{N\to\infty} \frac{1}{(2\pi\hbar)^{nN}} \int d^n r_1 \ldots d^n r_{N-1}\, d^n p_0 \ldots d^n p_{N-1}$

now take trace

$$\operatorname{tr} e^{-\frac{i}{\hbar}\hat{H}t} = \int d^n r_0 \langle \underline{r}_0 | e^{-\frac{i}{\hbar}\hat{H}t} | \underline{r}_0 \rangle$$

$$= \int \tilde{\mathcal{D}}[\underline{r}]\,\tilde{\mathcal{D}}[\underline{p}]\, \exp\left(\frac{i}{\hbar}\int_0^t [\underline{p}(t')\cdot\dot{\underline{r}}(t') - H(\underline{r}(t'),\underline{p}(t'))]\,dt'\right)$$

where $\int \tilde{\mathcal{D}}[\underline{r}]\,\tilde{\mathcal{D}}[\underline{p}]\ldots = \lim\limits_{N\to\infty} \frac{1}{(2\pi\hbar)^{nN}} \int d^n r_0 \ldots d^n r_{N-1}\, d^n p_0 \ldots d^n p_{N-1} \ldots$

conditions: $\underline{r}(t) = \underline{r}(0)$

$\underline{p}(t) = \underline{p}(0)$ can be added

H obtained from $\hat{H}$ by $\hat{\underline{r}}, \hat{\underline{p}} \to \underline{r}, \underline{p}$

In second quantisation

e.g. $\hat{H} = \sum_{i,j} H(i,j)\, a_i^\dagger a_j + \frac{1}{2} \sum_{i,j} \mathcal{U}^{int}(i,j)\, a_i^\dagger a_j^\dagger a_j a_i$

H obtained by $a_j, a_j^\dagger \to a_j, a_j^* \in \mathbb{C}$

$$\boxed{\operatorname{tr} e^{-\frac{i}{\hbar}\hat{H}t} = \int_{a_j(0)=a_j(t)} \mathcal{D}[a_1, a_2, \ldots] \exp\left(\int_0^t dt' \left[-\sum_j a_j^*(t')\,\dot{a}_j(t') - \frac{i}{\hbar} H(a_1(t'), a_2(t'), \ldots, a_1^*(t'), a_2^*(t'), \ldots)\right]\right)}$$

Motivation (heuristic):

analogy to harmonic oscillator $(m = \omega = 1)$

$$a_j(t') = \frac{1}{\sqrt{2\hbar}} \left(r_j(t') + i p_j(t') \right)$$

$$a_j^*(t') = \frac{1}{\sqrt{2\hbar}} \left(r_j(t') - i p_j(t') \right)$$

Commutator $[a_j, a_j^+] = 1$ due to $[\hat{r}_j, \hat{p}_j] = i\hbar$

Solve for $r_j(t'), p_j(t')$

$$r_j(t') = \sqrt{\frac{\hbar}{2}} \left(a_j(t') + a_j^*(t') \right)$$

$$p_j(t') = \sqrt{\frac{\hbar}{2}} \, \frac{1}{i} \left(a_j(t') - a_j^*(t') \right)$$

$$\frac{i}{\hbar}\int_0^t \sum_j p_j \dot{r}_j \, dt' = \frac{1}{2}\int_0^t \sum_j (a_j - a_j^*)(\dot{a}_j + \dot{a}_j^*) \, dt'$$

$$\int_0^t a_j \dot{a}_j \, dt' = \frac{1}{2} a_j^2 \Big|_0^t = 0$$

$$\int_0^t a_j^* \dot{a}_j^* \, dt' = \frac{1}{2} a_j^{*2} \Big|_0^t = 0$$

$$\int_0^t a_j \dot{a}_j^* \, dt' = a_j a_j^* \Big|_0^t - \int_0^t \dot{a}_j a_j^* \, dt'$$

So $\frac{i}{\hbar}\int_0^t \sum_j p_j \dot{r}_j = -\int_0^t \sum_j a_j^* \dot{a}_j \, dt'$

<u>Derivation</u>: using coherent states (see Altland & Simons book)

Continuum limit

$j \to x$ (in 1d)

$a_j(t') \to a(x,t')$

$$\mathrm{tr}\, e^{-\frac{i}{\hbar}\hat{H}t} = \int\limits_{\substack{a(x,t') \\ \text{with} \\ a(x,0)=a(x,t)}} D[a] \; \exp\Big(\int_0^t dt' \int dx \Big[-a^*(x,t')\,\dot{a}(x,t') - \frac{i}{\hbar} a^*(x,t')\Big(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)\Big) a(x,t) \Big] \Big)$$

without interaction

Applications

- can use perturbation theory
  e.g. for Bose-Hubbard model

$$\int D[a_1, a_2, \ldots] \exp\Big(-\int_0^t \sum_j a_j^*(t')\, \dot{a}_j(t')\, dt'$$

$$\underbrace{-\frac{i}{\hbar}\int_0^t \Big[-a_1^*(t')a_2(t') - a_2^*(t')a_1(t')}_{\text{quadratic}} \underbrace{+ \frac{U^{int}}{2}\sum_j a_j(t')^{*2} a_j(t')^2\Big]\Big)}_{\substack{\text{perturbation} \\ \text{(if } U^{int} \text{ is small)}}}$$

- when is action stationary?

$$\exp\left(\frac{i}{\hbar}\int_0^t \mathcal{L}\, dt'\right)$$

$$\mathcal{L} = -\frac{\hbar}{i}\sum_j a_j^* \dot{a}_j + a_1^* a_2 + a_2^* a_1 - \frac{U^{int}}{2}\sum_j a_j^{*2} a_j^2$$

action stationary if

$$\frac{\partial \mathcal{L}}{\partial a_j} = \frac{d}{dt'}\frac{\partial \mathcal{L}}{\partial \dot{a}_j} \qquad \frac{\partial \mathcal{L}}{\partial a_j^*} = \frac{d}{dt'}\frac{\partial \mathcal{L}}{\partial \dot{a}_j^*}$$

2nd eq gives

$$-\frac{\hbar}{i}\dot{a}_j + a_{j\pm 1} - U^{int} a_j^* a_j^2 = 0$$

$$i\hbar \dot{a}_j = -a_{j\pm 1} + U^{int}|a_j|^2 a_j$$

nonlinear Schrödinger equation (Gross-Pitaevski equation)