Wick theorem

for $\langle \ldots \rangle = \int d^n x \, \frac{1}{c} \, e^{\frac{i}{2} \underline{x}^T A \underline{x}} \ldots$

e.g. $\langle x_{k_1} x_{k_2} x_{k_3} x_{k_4} \rangle = \langle \overbrace{x_{k_1} x_{k_2}} \, \overbrace{x_{k_3} x_{k_4}} \rangle + \langle \overbrace{x_{k_1} x_{k_2} x_{k_3}}^{1\text{–}3} \! x_{k_4} \rangle_{\overbrace{k_2 \ldots k_4}} + \langle \overbrace{x_{k_1} \overbrace{x_{k_2} x_{k_3}} x_{k_4}} \rangle$

where $\overbrace{x_{k_i} x_{k_e}}$ gives $i(A^{-1})_{k_i k_e}$

harmonic oscillator

$$\frac{i}{\hbar} \int_0^t \left(\frac{1}{2} m \dot{x}(t')^2 - \frac{1}{2} m \omega^2 x(t')^2 \right) dt' = \frac{i}{2} \int_0^t x(t') \underbrace{\left(-\frac{m}{\hbar}\right)\left(\frac{\partial^2}{\partial t'^2} + \omega^2\right)}_{A} x(t') \, dt'$$

A^{-1} has integral kernel

$$G(t', t'') = -\frac{\hbar}{m \omega \sin \omega t} \begin{cases} \sin \omega t' \, \sin \omega (t'' - t) & \text{for } t' \leq t'' \\ \sin \omega t'' \, \sin \omega (t' - t) & \text{for } t' > t'' \end{cases}$$

Propagator

$$K_{harm}(0,0,t) = \int\limits_{x(0)=x(t)=0} D[x] \; \exp\left(\frac{i}{\hbar}\int_0^t \left[\frac{1}{2}m\dot{x}(t')^2 - \frac{1}{2}m\omega^2 x(t')^2\right]dt'\right) = c$$

$$K_{anh}(0,0,t) = \int\limits_{x(0)=x(t)=0} D[x] \; \exp\left(\frac{i}{\hbar}\int_0^t \left[\frac{1}{2}m\dot{x}(t')^2 - \frac{1}{2}m\omega^2 x(t')^2 - \varepsilon x(t')^4\right]dt'\right)$$

$$\langle \ldots \rangle = \int\limits_{x(0)=x(t)=0} D[x] \; \frac{1}{c} \exp\left(\frac{i}{\hbar}\int_0^t \left[\frac{1}{2}m\dot{x}(t')^2 - \frac{1}{2}m\omega^2 x(t')^2\right]dt'\right) \ldots$$

$$\left\langle \exp\left(-\frac{i\varepsilon}{\hbar}\int_0^t x(t')^4 \, dt'\right)\right\rangle = \frac{1}{c} K_{anh}(0,0,t)$$

$$K_{anh}(0,0,t) = K_{harm}(0,0,t)\left\langle \exp\left(-\frac{i\varepsilon}{\hbar}\int_0^t x(t')^4\, dt'\right)\right\rangle$$

$$= K_{harm}(0,0,t)\left\langle 1 - \frac{i\varepsilon}{\hbar}\int_0^t x(t')^4 dt' + \frac{1}{2}\left(-\frac{i\varepsilon}{\hbar}\int_0^t x(t')^4 dt'\right)^2 + O(\varepsilon^3)\right\rangle$$

$$= K_{harm}(0,0,t)\left(1 - \frac{i\varepsilon}{\hbar}\int_0^t dt' \langle x(t')^4\rangle + \frac{1}{2}\left(-\frac{i\varepsilon}{\hbar}\right)^2 \int_0^t dt' \int_0^t dt'' \langle x(t')^4 x(t'')^4\rangle + O(\varepsilon^3)\right)$$

linear term

$$\langle x(t')^4\rangle = \langle x(t')\,x(t')\,x(t')\,x(t')\rangle + \langle x(t')\,x(t')\,x(t')\,x(t')\rangle$$

$$+ \langle x(t')\,x(t')\,x(t')\,x(t')\rangle$$

discrete case: $x_{k_i} \; x_{k_l}$ gives $i\,(A^{-1})_{k_i k_l}$

here: $x(t')\; x(t'')$ gives $i\,G(t',t'')$

$$\langle x(t')^4\rangle = 3\,(i\,G(t',t'))^2$$

where $G(t',t') = -\dfrac{\hbar \sin\omega t' \sin\omega(t'-t)}{m\omega \sin\omega t}$

$$K_{anh}(0,0,t) = K_{harm}(0,0,t)\left(1 + \frac{3i\varepsilon}{\hbar}\int_0^t dt'\,(G(t',t'))^2 + O(\varepsilon^2)\right)$$

Ground state energy

$$\langle 0 | e^{-\frac{i}{\hbar}\hat{H}t} | 0 \rangle \xrightarrow[\text{replace } \frac{i}{\hbar}t \to \beta]{} \langle 0 | e^{-\beta \hat{H}} | 0 \rangle \underset{\beta \to \infty}{\propto} e^{-\beta E_0}$$

replace $\frac{i}{\hbar} t \to \beta$

$$\langle 0 | e^{-\beta \hat{H}_{anh}} | 0 \rangle = \langle 0 | e^{-\beta \hat{H}_{harm}} | 0 \rangle$$

$$\cdot \left(1 + 3\varepsilon \int_0^\beta d\beta' \, G\left(\tfrac{\hbar}{i}\beta', \tfrac{\hbar}{i}\beta'\right)^2 + O(\varepsilon^2) \right)$$

$$G\left(\tfrac{\hbar}{i}\beta', \tfrac{\hbar}{i}\beta'\right) = -\frac{\hbar}{m\omega} \frac{\sin\left(\omega \frac{\hbar}{i}\beta'\right) \sin\left(\omega \frac{\hbar}{i}(\beta' - \beta)\right)}{\sin\left(\omega \frac{\hbar}{i}\beta\right)}$$

$$\sin\left(\omega \tfrac{\hbar}{i}\beta\right) = \frac{1}{2i}\left(e^{i\omega\frac{\hbar}{i}\beta} - e^{-i\omega\frac{\hbar}{i}\beta}\right) \underset{\beta \to \infty}{\simeq} \frac{1}{2i} e^{\omega\hbar\beta}$$

Similarly:

$$\sin\left(\omega\frac{\hbar}{i}\beta'\right) \simeq \frac{1}{2i} e^{\omega\hbar\beta'}$$

$$-\sin\left(\omega\frac{\hbar}{i}(\beta'-\beta)\right) = \sin\left(\omega\frac{\hbar}{i}(\beta-\beta')\right) \simeq \frac{1}{2i} e^{\omega\hbar(\beta-\beta')}$$

So

$$G\left(\frac{\hbar}{i}\beta', \frac{\hbar}{i}\beta'\right) \simeq \frac{\hbar}{2im\omega} \underbrace{\frac{e^{\omega\hbar\beta'} e^{\omega\hbar(\beta-\beta')}}{e^{\omega\hbar\beta}}}_{=1}$$

$$\langle 0| e^{-\beta\hat{H}_{anh}} |0\rangle \simeq \langle 0| e^{-\beta\hat{H}_{harm}} |0\rangle \left(1 - \frac{3}{4}\varepsilon\left(\frac{\hbar}{m\omega}\right)^2\beta\right)$$

$$\propto e^{-\beta\frac{1}{2}\hbar\omega} e^{-\beta\frac{3}{4}\varepsilon\left(\frac{\hbar}{m\omega}\right)^2}$$

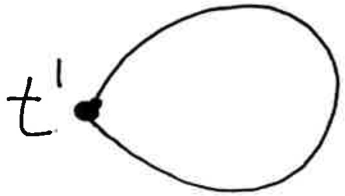
$$\boxed{E_0 = \frac{1}{2}\hbar\omega + \frac{3}{4}\varepsilon\left(\frac{\hbar}{m\omega}\right)^2 + O(\varepsilon^2)}$$

Feynman diagrams

$\overline{x(t') \quad x(t'')}$

$iG(t',t'')$

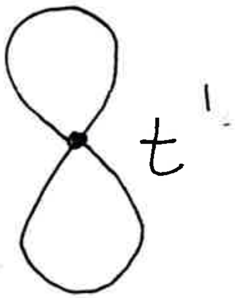
$\overline{x(t') \quad x(t')}$



$iG(t',t')$

t' with more than one end of a line attached are integrated over

$$\int dt' \langle x(t')^4 \rangle = 3$$



↑ multiplicity

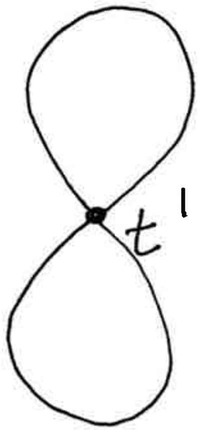
ε^2 contribution

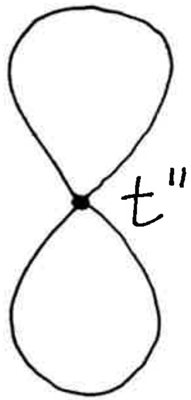
$$\int dt' \int dt'' \langle x(t')^4 \, x(t'')^4 \rangle$$

(a) all $x(t')$ contracted among each other, same for $x(t'')$

e.g. $\int dt' \int dt'' \langle x(t') x(t') x(t') x(t') x(t'') x(t'') x(t'') x(t'') \rangle$

$= \int dt' \int dt'' \, (iG(t',t'))^2 \, (iG(t'',t''))^2$



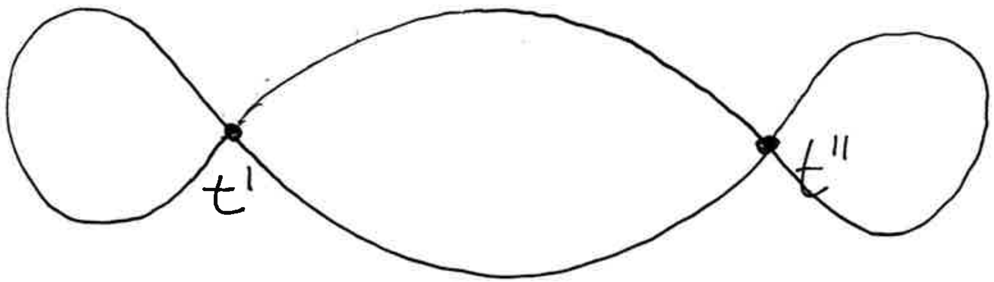


multiplicity: 3 ways to contract $x(t')$
3 ways to contract $x(t'')$
altogether 9

(b) two $x(t')$ contracted with $x(t'')$

e.g. $\int dt' \int dt'' \langle x(t')\, x(t')\, x(t')\, x(t')\, x(t'')\, x(t'')\, x(t'')\, x(t'') \rangle$

$= \int dt' \int dt'' \, (iG(t',t''))^2 \, iG(t',t') \, iG(t'',t'')$



multiplicity: $\binom{4}{2} = 6$ ways of dividing up $x(t')$

same for $x(t'')$

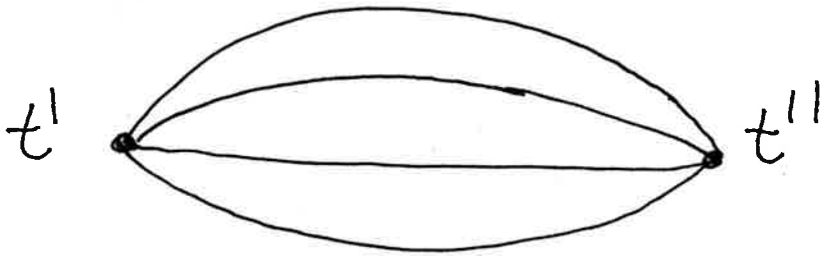
2 ways of contracting $x(t')$ & $x(t'')$

altogether 72

(c) all $x(t')$ contracted with $x(t'')$

e.g. $\int dt' \int dt'' \langle x(t')\, x(t')\, x(t')\, x(t')\, x(t'')\, x(t'')\, x(t'')\, x(t'') \rangle$

$= \int dt' \int dt'' \left(iG(t',t'') \right)^4$



multiplicity: $4! = \mathbf{24}$ ways of ordering $x(t'')$
(to decide which $x(t')$ they are connected to)

4 Second quantisation

4.1 Two particles

Hamiltonian e.g. $\hat{H} = \frac{\hat{\underline{p}}_1^2}{2m} + \mathcal{U}(\underline{r}_1) + \frac{\hat{\underline{p}}_2^2}{2m} + \mathcal{U}(\underline{r}_2) + \mathcal{U}^{int}(\underline{r}_1, \underline{r}_2)$

$\uparrow$ e.g. $\frac{a}{|\underline{r}_1 - \underline{r}_2|}$

Wavefunction $\psi(\underline{r}_1, \underline{r}_2)$

basis for single-particle wavef. $\varphi_i(\underline{r})$ $\quad |i\rangle$

for two-particle wavef. $\varphi_i(\underline{r}_1)\varphi_j(\underline{r}_2)$ $\quad |i\rangle \otimes |j\rangle$

$= |i\rangle |j\rangle$

Indistinguishable particles

can't distinguish whether particle 1 found at $\underline{r}_1$ and particle 2 found at $\underline{r}_2$ or the other way around

$$|\psi(\underline{r}_1,\underline{r}_2)|^2 = |\psi(\underline{r}_2,\underline{r}_1)|^2$$

$$\Rightarrow \psi(\underline{r}_2,\underline{r}_1) = e^{i\varphi}\,\psi(\underline{r}_1,\underline{r}_2)$$

law of nature:
- $e^{i\varphi} = 1$ for **bosons** (e.g. photons)
- $e^{i\varphi} = -1$ for **fermions** (e.g. electrons, protons)
- $e^{i\varphi} \neq 1,-1$ impossible for fundamental particles

Spin: multi-comp. wavefunctions $\psi_\sigma(\underline{r}) = \psi(\sigma, \underline{r})$

for spin systems replace $\underline{r} \to (\sigma, \underline{r})$ in the following

Wave functions: $\psi(\underline{r}_1, \underline{r}_2)$ with $\psi(\underline{r}_2, \underline{r}_1) = \pm\, \psi(\underline{r}_1, \underline{r}_2)$

basis: $\psi_{ij}(\underline{r}_1, \underline{r}_2) = C\left(\psi_i(\underline{r}_1)\,\psi_j(\underline{r}_2) \pm \psi_j(\underline{r}_1)\,\psi_i(\underline{r}_2)\right)$

(+: bosons; −: fermions)

↑ 1 particle in state i, 1 particle in state j

C: normalisation

$$|i,j\rangle = C\left(|i\rangle\,|j\rangle \pm |j\rangle\,|i\rangle\right)$$

for fermions:

$$|i,i\rangle = 0$$

no two fermions can be in the same single particle state (**Pauli exclusion principle**)

normalisation :

$$\int \varphi_i^*(\underline{r})\, \varphi_{i'}(\underline{r})\, d^n r = \delta_{ii'}$$

$$\int \left(\varphi_i(\underline{r}_1)\, \varphi_j(\underline{r}_2)\right)^* \varphi_{i'}(\underline{r}_1)\, \varphi_{j'}(\underline{r}_2)\, d^n r_1\, d^n r_2 = \delta_{ii'}\,\delta_{jj'}$$

$$1 \overset{!}{=} \int \left|\varphi_{ij}(\underline{r}_1, \underline{r}_2)\right|^2 d^n r_1\, d^n r_2$$

$$= |C|^2 \int \left(\varphi_i(\underline{r}_1)\varphi_j(\underline{r}_2) \pm \varphi_j(\underline{r}_1)\, \varphi_i(\underline{r}_2)\right)^*$$

$$\left(\varphi_i(\underline{r}_1)\varphi_j(\underline{r}_2) \pm \varphi_j(\underline{r}_1)\, \varphi_i(\underline{r}_2)\right) d^n r_1\, d^n r_2$$

$$\underset{i \neq j}{=} |C|^2 \, (1 + 1)$$

$$\Rightarrow |C| = \frac{1}{\sqrt{2}}, \quad \text{choose } C = \frac{1}{\sqrt{2}}$$