Tutorial 6/11/2014

{Statistical Physics}

Second Quantization Formalism

- very useful for many-body quantum systems! (circumvents complicated many-body wavefunction symmetrization/antisymmetrization hassle)
  - → simplifies treatment of interparticle interactions...
  - → ...of systems where particle number is not conserved...
  - → ...and is used in many (other) important parts of physics!
- works in Fock space

$$\mathcal{F} = \bigoplus_{n=0}^{\infty} Q_n$$ ← Hilbert spaces of different ptcl. #.

- usually here represents a many-body state (at least when we work without interactions) in terms of occupation number states

$$|n_{\nu_1}, n_{\nu_2}, \dots\rangle$$

# of ptcls in states $\nu_1, \nu_2, \dots$

(NOTE: We can (and will) also work with $|\vec{r}_1, s_1; \vec{r}_2, s_2; \dots\rangle$ & field operators $\hat{\Psi}_s(\vec{r}), \hat{\Psi}_s^+(\vec{r})$)

$\hat{\ }$ = operator (but it's unreasonable to ask for consistent usage ☺)

and creation & annihilation operators

$$\hat{a}_\nu : Q_n \to Q_{n-1}$$
$$\hat{a}_\nu^+ : Q_n \to Q_{n+1}$$

with

$$\hat{a}_\nu |n_1, \dots n_\nu, \dots\rangle = \sqrt{n_\nu}\, |n_{\nu_1}, \dots n_\nu - 1, \dots\rangle$$
$$\hat{a}_\nu^+ |n_1, \dots n_\nu, \dots\rangle = \sqrt{n_\nu + 1}\, |n_{\nu_1}, \dots n_\nu + 1, \dots\rangle$$

⇒ number operator

$\hat{n}_\nu = \hat{a}_\nu^+ \hat{a}_\nu$ has eigenstates $|n_{\nu_1}, \dots n_\nu \dots\rangle$ with EV n_ν

For non-interacting particles, these states are also the Hamiltonian eigenstates!

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Useful properties of $a_\nu, a_\nu^\dagger$:

FERMIONS

$$\{\hat{a}_\nu, \hat{a}_{\nu'}^\dagger\} = \delta_{\nu\nu'}$$

$$\{\hat{a}_\nu, \hat{a}_{\nu'}\} = \{a_\nu^\dagger, a_{\nu'}^\dagger\} = 0$$

$$\hookrightarrow \hat{a}_\nu^\dagger \hat{a}_\nu^\dagger = \hat{a}_\nu \hat{a}_\nu = 0$$

BOSONS

$$[\hat{a}_\nu, a_{\nu'}^\dagger] = \delta_{\nu\nu'}$$

$$[\hat{a}_\nu, \hat{a}_{\nu'}] = [\hat{a}_\nu^\dagger, \hat{a}_{\nu'}^\dagger] = 0$$

BOTH

For $\mathcal{H} = \sum_k \hat{a}_k^\dagger \hat{a}_k \epsilon_k$:

these are in particular useful for thermal averages!

$$\begin{cases} e^{-\beta\mathcal{H}} \hat{a}_k^\dagger e^{\beta\mathcal{H}} = e^{-\beta\epsilon_k} \hat{a}_k^\dagger \\ e^{\beta\mu\hat{N}} \hat{a}_k^\dagger e^{-\beta\mu\hat{N}} = e^{\beta\mu} \hat{a}_k^\dagger \end{cases}$$

For any eigenstate $|\phi\rangle$ of $\mathcal{H}$,

$$\langle\phi|\hat{a}_\nu^\dagger|\phi\rangle = \langle\phi|\hat{a}_\nu|\phi\rangle = \langle\phi|a_\nu^\dagger a_{\nu'}^\dagger|\phi\rangle = \ldots = 0$$

$$\langle\phi|a_\nu^\dagger a_{\nu'}|\phi\rangle = \delta_{\nu\nu'} n_\nu .$$

Thermal averages:

In equilibrium, the system will be (density matrix formalism!) in the state

$$\rho = \frac{1}{Z} e^{-\beta\mathcal{H}'} \longleftarrow \mathcal{H}' = \mathcal{H} - \mu\hat{N}$$

(grand-canonical ensemble)

either true situation or convenient model (easy partition function & analysis)

$\Rightarrow$ calculate average of operator A as

$$\langle A\rangle = \frac{1}{Z} \mathrm{tr}(e^{-\beta\mathcal{H}'} A)$$

$\rightarrow$ this can be tedius ... need to make full use of the properties above!

Example:

(1) **BOSONS**

you'll look at this object for correlation functions

$$\langle a_k^\dagger a_q^\dagger a_{q'} a_{k'}\rangle = \frac{1}{Z}\mathrm{tr}\left[e^{-\beta\mathcal{H}'} a_k^\dagger a_q^\dagger a_{q'} a_{k'}\right] = \frac{1}{Z}\mathrm{tr}\left(e^{-\beta\mathcal{H}'} a_k^\dagger e^{\beta\mathcal{H}'} e^{-\beta\mathcal{H}'} a_q^\dagger a_{q'} a_{k'}\right)$$

$$= \frac{e^{-\beta(\epsilon_k-\mu)}}{Z}\mathrm{tr}\left(e^{-\beta\mathcal{H}'} a_q^\dagger a_{q'} a_{k'} a_k^\dagger\right) = \frac{e^{-\beta(\epsilon_k-\mu)}}{Z}\mathrm{tr}\left(e^{-\beta\mathcal{H}'} a_q^\dagger a_{q'} (\delta_{kk'} + a_k^\dagger a_{k'})\right)$$

$$= \frac{e^{-\beta(\epsilon_k-\mu)}}{Z}\left[Z\langle n_q\rangle \delta_{qq'}\delta_{kk'} + \mathrm{tr}\left(e^{-\beta\mathcal{H}'} a_q^\dagger (\delta_{kq'} + a_k^\dagger a_{q'}) a_{k'}\right)\right)$$

$$= \frac{e^{-\beta(\epsilon_k-\mu)}}{\cancel{Z}}\left[\langle n_q\rangle \delta_{qq'}\delta_{kk'} + \langle n_q\rangle \delta_{kq'}\delta_{qk'}\right] + \frac{e^{-\beta(\epsilon_k-\mu)}}{\cancel{Z}}\langle a_k^\dagger a_q^\dagger a_{q'} a_{k'}\rangle$$

$$\Rightarrow \langle a_k^\dagger a_q^\dagger a_{q'} a_{k'}\rangle = \frac{1}{e^{\beta(\epsilon_k-\mu)}-1}\left(\langle n_q\rangle(\delta_{qq'}\delta_{kk'} + \delta_{kq'}\delta_{qk'})\right) = \langle n_k\rangle\langle n_q\rangle(\delta_{qq'}\delta_{kk'} + \delta_{kq'}\delta_{qk'})$$

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② (BOSONS)

$$\langle n_k n_q \rangle = \frac{1}{Z}\, \mathrm{tr}\left(e^{-\beta \mathcal{H}'} a_k^+ a_k a_q^+ a_q\right) = \frac{e^{-\beta(\epsilon_k-\mu)}}{Z}\, \mathrm{tr}\left(e^{-\beta\mathcal{H}'} a_k a_q^+ a_q a_k^+\right)$$

$$= \frac{e^{-\beta(\epsilon_k-\mu)}}{Z}\, \mathrm{tr}\left(e^{-\beta\mathcal{H}'} a_k a_k^+ \left(\delta_{kk'} + a_q^+ a_q\right)\right) = \ldots \text{(similar modulations)}$$

OR use previous relation to get

$$\langle n_k n_q\rangle = \langle a_k^+ a_k a_q^+ a_q\rangle = \langle a_k^+ (a_q^+ a_k + \delta_{kq}) a_q\rangle = \langle n_k\rangle \delta_{kq} + \langle n_k\rangle\langle n_q\rangle(1+\delta_{kq})$$

FERMIONS → very similar, just remember

- swapping $a_k a_q$ or $a_k^+ a_q^+$ gives − sign!
- to include spin! (or include it into the label k)

CONSISTENCY CHECK:

There's one more thing we can do: go through different cases!

E.g. for $\langle a_k^+ a_q^+ a_{q'} a_{k'}\rangle$

1) $k=k',\ q=q',\ k\neq q \Rightarrow \langle n_k n_q\rangle$
2) $k=q',\ k'=q,\ k\neq q \Rightarrow \langle n_k n_q\rangle$
3) $k=q=k'=q' \Rightarrow \sum_{\{n\}} p_{\{\}} \langle n_{k_1} \ldots n_k \ldots | \sqrt{n_k}\sqrt{n_k-1}\sqrt{n_k-1}\sqrt{n_k}\, | n_{k_1} \ldots n_k\rangle = \langle n_k^2 -$

(all other cases will be 0 because $\langle\ldots\rangle$ is really a $\sum_\phi p_\phi \langle\phi|\ldots|\phi\rangle$

occupation numbers states $|\phi\rangle = |n_{k_1} n_{k_2} \ldots\rangle$

$$\Rightarrow \langle a_k^+ a_q^+ a_{q'} a_{k'}\rangle = (1-\delta_{kq})\langle n_k n_q\rangle\left(\delta_{kk'}\delta_{qq'} + \delta_{kq'}\delta_{qk'}\right) + \delta_{kq}\delta_{kk'}\delta_{qq'}\langle n_k^2 - n_k\rangle$$

⇝ really, use what you feel most comfortable with! :)

Application: Particle numbers fluctuations in bosons & fermions

Recall:

$$\langle n_k n_q\rangle = \delta_{kq}\,(1 \pm \langle n_k\rangle)\langle n_k\rangle + \langle n_k\rangle\langle n_q\rangle.$$

(+ Bosons, − Fermions)

Now

$$\text{fluct}(k) = \boxed{\langle n_k^2\rangle - \langle n_k\rangle^2 = \langle n_k\rangle \pm \langle n_k\rangle^2}$$

with

$$\langle n_k\rangle = \frac{1}{e^{\beta(\epsilon_k-\mu)} \mp 1} \Rightarrow \boxed{\langle n_k^2\rangle - \langle n_k\rangle^2 = \frac{e^{\beta(\epsilon_k-\mu)}}{\left(e^{\beta(\epsilon_k-\mu)} \mp 1\right)^2}}$$

fluctuations for individual mode

What about

$\langle N^2\rangle - \langle N\rangle^2$? With $N = \sum_k n_k$

$$\Rightarrow \langle N^2\rangle - \langle N\rangle^2 = \left\langle\sum_{kq} \langle n_k n_q\right\rangle - \left(\sum_k \langle n_k\rangle\right)^2 = \left(\sum_{kq} \langle n_k\rangle(1\pm\langle n_k\rangle)\delta_{kq} + \overbrace{\langle n_k\rangle\langle n_q\rangle\right) - \sum_{kq}\langle n_k\rangle\langle n_q\rangle}^{0} = \sum_k \langle n_k\rangle(1\pm\langle n_k\rangle)$$

$$= \sum \text{fluct}(k)$$ → sum of single mod...

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Classical Limit:

($e^{\beta\mu} \ll 1$)

($e^{-\beta(\epsilon_k-\mu)}$ small)

$$\langle n_k^2\rangle - \langle n_k\rangle^2 = \langle n_k\rangle \underset{\text{Fermions}}{\overset{\text{Bosons}}{\pm}} \langle n_k\rangle\langle n_k\rangle$$

$$= \frac{e^{\beta(\epsilon_k-\mu)}}{(e^{\beta(\epsilon_k-\mu)} \mp 1)^2}$$

$$\approx \left(1 \pm e^{-\beta(\epsilon_k-\mu)}\right)\left(1 \pm e^{-\beta(\epsilon_k-\mu)}\right) e^{-\beta(\epsilon_k-\mu)}$$

$$\approx e^{-\beta(\epsilon_k-\mu)} \pm 2e^{-2\beta(\epsilon_k-\mu)}$$

In this limit, also

$$\langle n_k\rangle \approx e^{-\beta(\epsilon_k-\mu)}\left(1 \pm e^{-\beta(\epsilon_k-\mu)}\right)$$

and so

$$\boxed{\langle n_k^2\rangle - \langle n_k\rangle^2 \approx \langle n_k\rangle \pm e^{-2\beta(\epsilon_k-\mu)}}$$

- to first order, Bosons & Fermions give the same result as expected ✓
- first correction increases fluctuations for Bosons, decreases for Fermions

TOTAL FLUCTUATIONS

$$\langle N^2\rangle - \langle N\rangle^2 = \sum_k \langle n_k^2\rangle - \langle n_k\rangle^2 \approx \langle N\rangle \pm \sum_k e^{-2\beta(\epsilon_k-\mu)}$$

$$\Rightarrow K_T = \underbrace{\frac{V}{k_B T}}_{\text{V/N}} \frac{\langle N^2\rangle - \langle N\rangle^2}{\langle N\rangle} \approx \underbrace{\frac{V}{k_B T}}_{\text{classical result}} \pm \frac{\sum_k e^{-2\beta(\epsilon_k-\mu)}}{\langle N\rangle}$$

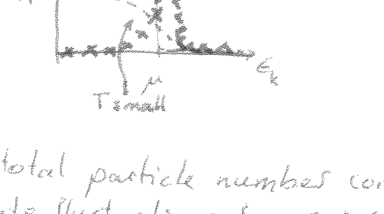
First correction:
+ for Bosons
− for Fermions
(as we have seen already in lecture)
↳ different expression though

Small temperatures:

FERMIONS

$T \to 0 \Rightarrow$ $\epsilon_k > \mu$: Fluctuations $\to 0$, $n_k \to 0$

$\epsilon_k < \mu$: Fluctuations $\to 0$, $n_k \to 1$



Use $\langle n_k^2\rangle - \langle n_k\rangle^2 = \frac{e^{\beta(\epsilon_k-\mu)}}{(e^{\beta(\epsilon_k-\mu)} \mp 1)^2}$ — Bosons / Fermions

BOSONS For BEC we left total particle number conserved! So we have to be a bit careful what we mean...

→ could calculate fluctuations for $\epsilon_k > \epsilon_0$: those will $\to 0$ as $T \to 0$

(in this sense also for BEC fluctuations $\to 0$)