BCS-type theory in canonical ensembles

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Contents :

I. Introduction

What is 'phase transition'?

infinite systems → well-established
↕
semi-classical

finite systems → ?
↕
fully quantal
(⇒ no transition due to quant. fluctuation?)

spontaneous symmetry breakdown $\Longleftrightarrow$ conservation law (*e.g.* particle #)
↔ phase transition ?

Note: "phase" ··· usually, semi-classical concept!

Questions:
(i) what roles conservation laws play?
(ii) how 'phase transition' develops as the particle-number increases?

Phases in atomic nuclei $\leftarrow$ mean-field (*i.e.* semi-classical) picture

- deformed shape *vs.* spherical shape
- superfluid *vs.* normal fluid

'nuclear temperature' $\leftrightarrow$ (average) excitation energy

$\rightarrow$ statistical properties

cf. astrophysical environment

$\rightarrow$ canonical ensemble treatment

for increasing T $\rightarrow$ phase transition ?

T : continuous parameter
non-linear contribution to free energy

signature of 'phase transition' $\rightarrow$ washed out by quantum fluctuations
(a part of quant. fluc. $\rightarrow$ restoring symmetry)

Superfluidity (or superconductivity) in finite fermionic systems

e.g. atomic nuclei, ultrasmall metallic grains

$\leftrightarrow$ breaking of n conservation ($U(1)$ gauge sym.) ($n:$ particle number)

$\leftarrow$ BCS or HFB theory

in practice, n conservation should be maintained

$\begin{cases} \text{sym. breaking — artifact (due to MF approx.)} \\ \Leftrightarrow \text{ sym. restored via quant. fluc.} \end{cases}$

$\Rightarrow$ a good example to study

(i) role of conservation laws & (ii) how 'phase transition' develops

in finite systems

II. BCS-type theory in canonical ensembles — formalism

finite-T BCS theory :

trial statistical operator $w_{\rm exact} = \dfrac{e^{-H/T}}{{\rm Tr}_{\rm C}(e^{-H/T})} \quad \rightarrow \quad w_{\rm G} = \dfrac{e^{-H_0/T}}{{\rm Tr}(e^{-H_0/T})}\,; \qquad H_0 = \sum_k \varepsilon_k \alpha_k^\dagger \alpha_k$

$\Leftrightarrow$ **Bogoliubov tr.** $\quad c_k^\dagger = u_k \alpha_k^\dagger - v_k \alpha_{\bar{k}}$

free energy $\quad F_{\rm G} = E_{\rm G} - TS_{\rm G}\,; \qquad E_{\rm G} = {\rm Tr}(w_{\rm G} H)\,, \quad S_{\rm G} = -{\rm Tr}(w_{\rm G} \ln w_{\rm G})$

Peierls inequality $F_{\rm G} \geq F_{\rm exact} \quad \Rightarrow$ **variation of $F_{\rm G}$ with respect to** (v_k, ε_k)

for a given T under ${\rm Tr}(w_{\rm G} N) = n$

$\cdots$ **'GCE-BCS' theory**

(cf. $\varepsilon_k \leftrightarrow f_k = 1/(e^{\varepsilon_k/T} + 1)$**)**

GCE $\xrightarrow[n\ \text{proj.}]{}$ **CE** $\qquad$ n **proj. op.** $\quad P_n = \dfrac{1}{2\pi}\displaystyle\int_0^{2\pi} e^{-i\varphi(N-n)} d\varphi$

$$w_{\rm C} = \frac{P_n e^{-H_0/T}}{{\rm Tr}(P_n e^{-H_0/T})} \quad \rightarrow \quad F_{\rm C} = E_{\rm C} - TS_{\rm C}\ (\geq F_{\rm exact})\,; \quad E_{\rm C} = {\rm Tr}(w_{\rm C} H)\,, \quad S_{\rm C} = -{\rm Tr}(w_{\rm C} \ln w_{\rm C})$$

however, $[P_n, H_0] \neq 0 \quad \rightarrow \quad S_{\rm C}$ **not tractable !**

further approx. of entropy : Ref. : K. Tanabe & H.N., P.R.C 71, 024314 ('05)

$$\tilde{F}_{\rm C} = E_{\rm C} - T\tilde{S}_{\rm C}\,; \qquad \tilde{S}_{\rm C} = \frac{1}{T}\frac{\mathrm{Tr}(e^{-H_0/T}H_0P_n)}{\mathrm{Tr}(e^{-H_0/T}P_n)} + \ln \mathrm{Tr}(e^{-H_0/T}P_n)$$

$\leftrightarrow$ **partially commuting P_n & H_0**

Peierls inequality $\tilde{F}_{\rm C} \geq F_{\rm C} \geq F_{\rm exact}$ $\Rightarrow$ **variation of $\tilde{F}_{\rm C}$ with respect to (v_k, f_k)**

for a given n & T

$\cdots$ **'CE-BCS' theory**

variational eq. with respect to v_k :

$$\frac{\delta\tilde{F}_{\rm C}}{\delta f_k} = 0 \;\rightarrow\; \sum_{k'} \varepsilon_{k'}\frac{\partial f^{\rm C}_{k'}}{\partial f_k} = \cdots \qquad \textbf{(coupled eq.)}$$

$$\frac{\delta\tilde{F}_{\rm C}}{\delta v_k} = 0 \;\rightarrow\; v_k^2 = \frac{1}{2}\left(1 - \frac{\tilde{\varepsilon}_k}{\sqrt{\tilde{\varepsilon}_k^2 + \tilde{\Delta}_k^2}}\right); \qquad \tilde{\Delta}_k \equiv \frac{1}{2}\Big[(\Delta_k^\varphi e^{-i\varphi} + \bar{\Delta}_k^\varphi e^{i\varphi})\}/\zeta_k^\varphi\Big]_\varphi\,, \qquad \tilde{\varepsilon}_k = \cdots \neq \varepsilon_k\,;$$

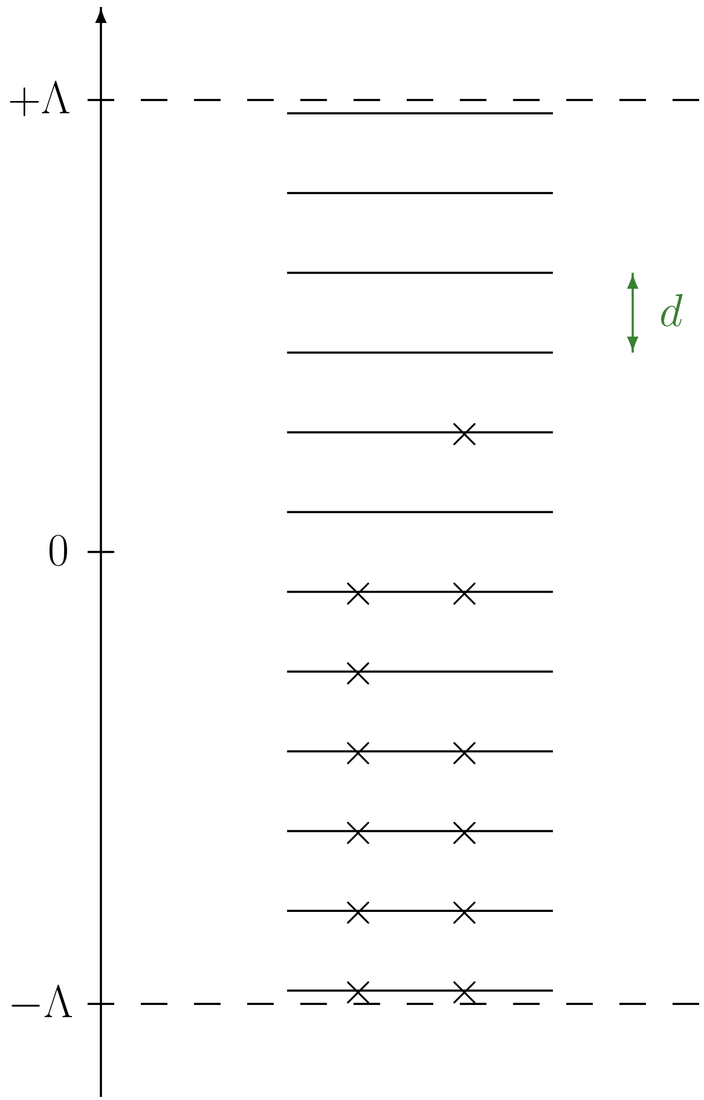
$$\big[X\big]_\varphi = \frac{\int d\Phi\, X}{\int d\Phi}\,, \qquad d\Phi = e^{i\varphi(n-\Omega)}\Big(\prod_{k>0}\zeta_k^\varphi\Big)d\varphi\,, \qquad w^\varphi = \frac{e^{-i\varphi N}e^{-H_0/T}}{\mathrm{Tr}(e^{-i\varphi N}e^{-H_0/T})}\,,$$

$$E^\varphi = \mathrm{Tr}(w^\varphi H)\,, \qquad \kappa_k^\varphi = \mathrm{Tr}(w^\varphi c_{\bar{k}}c_k)\,, \qquad \bar{\kappa}_k^\varphi = \mathrm{Tr}(w^\varphi c_k^\dagger c_{\bar{k}}^\dagger)\,,$$

$$-\Delta_k^\varphi = \frac{\delta E^\varphi}{\delta\bar{\kappa}_k^\varphi}\,, \qquad -\bar{\Delta}_k^\varphi = \frac{\delta E^\varphi}{\delta\kappa_k^\varphi}$$

$$\begin{cases} T = 0 & \Rightarrow\ n\text{-proj. BCS at zero } T \\ d\Phi = \delta(\varphi)\,d\varphi & \Rightarrow\ \text{GCE-BCS} \\ \int d\varphi \rightarrow \sum_{\varphi=0,\pi} & \Rightarrow\ \pi_n\text{-proj. BCS} \end{cases}$$

III. Numerical example in schematic models



- **s.p. levels** $\cdots$

  equi-distant with cut-off

  2-fold degeneracy $(t_k = t_{\bar{k}})$
- **half-filled** $(n = \Omega)$
- **constant pairing**

$$H = \sum_k t_k N_k - g\, B^\dagger B\,; \qquad B \equiv \sum_{k>0} c_{\bar{k}} c_k$$

- Δ_0 **: pairing gap in GCE-BCS at** $T = 0$

  $\Delta_0 = 1 \to g$ **(& energy scale)**

'gap' parameter ?

— order parameter in GCE-BCS

$$\Delta_{\rm G} = g\,\langle B\rangle_{\rm G}$$

$$\leftrightarrow \begin{cases} \tilde{\Delta}_k \\ \Delta_{\rm C}^{\rm av} \equiv g\sqrt{\langle B^\dagger B\rangle_{\rm C} - \sum_{k>0}\langle N_k\rangle_{\rm C}\,\langle N_{\bar{k}}\rangle_{\rm C}} \end{cases}$$

$$\begin{pmatrix} \langle\mathcal{O}\rangle_{\rm G} & \cdots & \textbf{GCE-BCS} \\ \langle\mathcal{O}\rangle_{\rm C} & \cdots & \textbf{CE-BCS} \\ \langle\mathcal{O}\rangle_{\pi} & \cdots & \pi_n\textbf{-proj. BCS} \end{pmatrix}$$

$n = 10$ $\Delta_{\rm G}$: (dashed green) $\Delta_{\rm C}^{\rm av}$: (solid green)

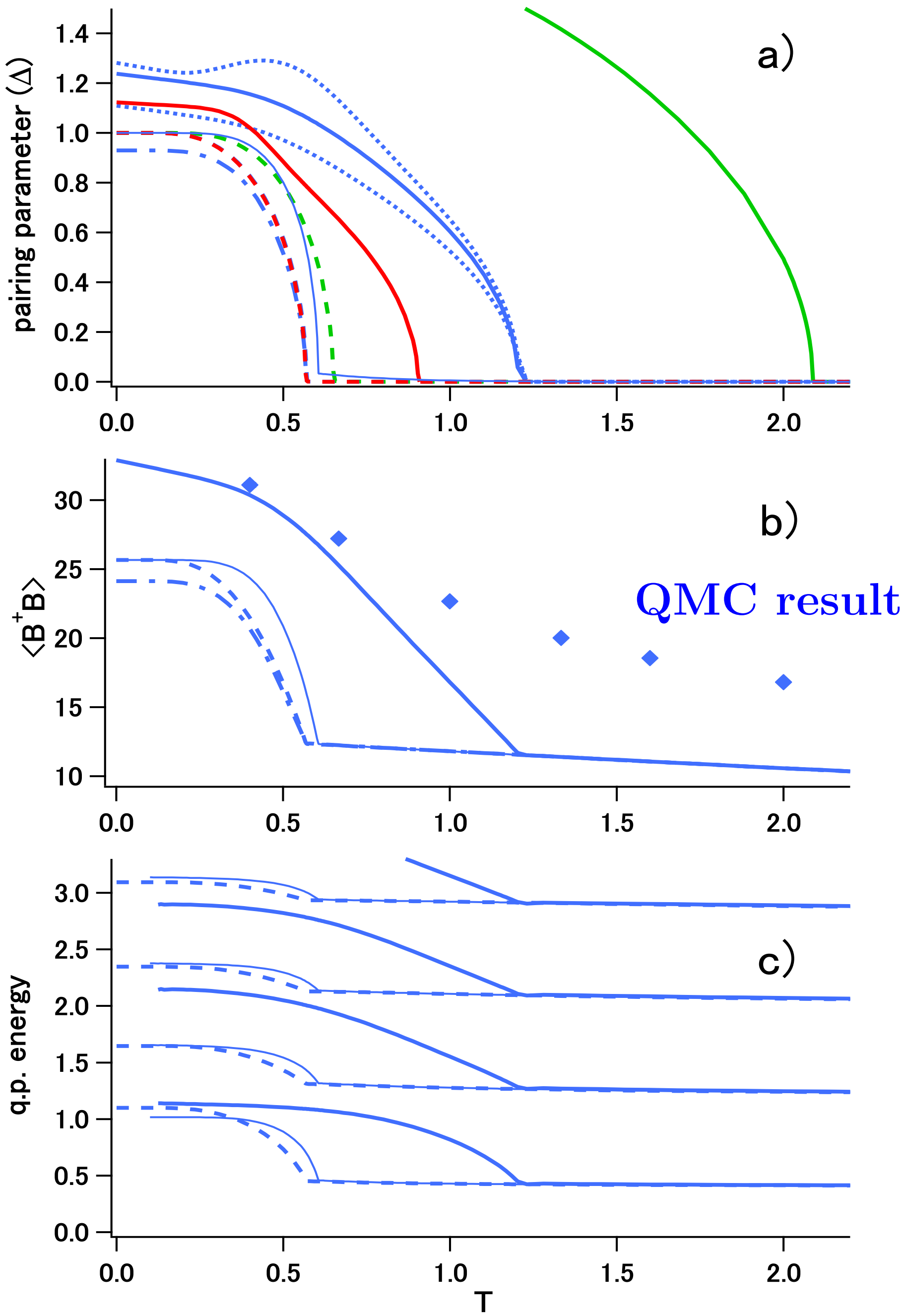
$n = 26$ $\Delta_{\rm G}$: (dashed blue) $\Delta_{\rm C}^{\rm av}$: (solid blue)

$\Delta_{\pi}^{\rm av}$: (thin solid blue) $\tilde{\Delta}_k$: (dotted blue)

$\Delta_{\rm C'}^{\rm av}$: (dash-dot blue)

$n = 56$ $\Delta_{\rm G}$: (dashed red) $\Delta_{\rm C}^{\rm av}$: (solid red)

$$\langle\mathcal{O}\rangle_{\rm C'} \equiv \langle\mathcal{O}P_n\rangle_{\rm G}\ (\textit{\textbf{i.e.}}\ \textbf{VBP}) \rightarrow \Delta_{\rm C'}^{\rm av}$$



specific heat ?

$$C = \frac{d\langle H \rangle}{dT} \quad \rightarrow \quad C/n$$

discontinuity in C

$\leftrightarrow$ **'phase transition'**

$\Rightarrow$ **in CE :**

- **'transition' remains**
- **$T^{\rm cr}$ shifted up**

why ? $\leftarrow$ **q.p. #** $\langle \mathcal{N} \rangle$; $\quad \mathcal{N} = \sum_k \alpha_k^\dagger \alpha_k$

CE $\cdots$ **reduced # of excited states**

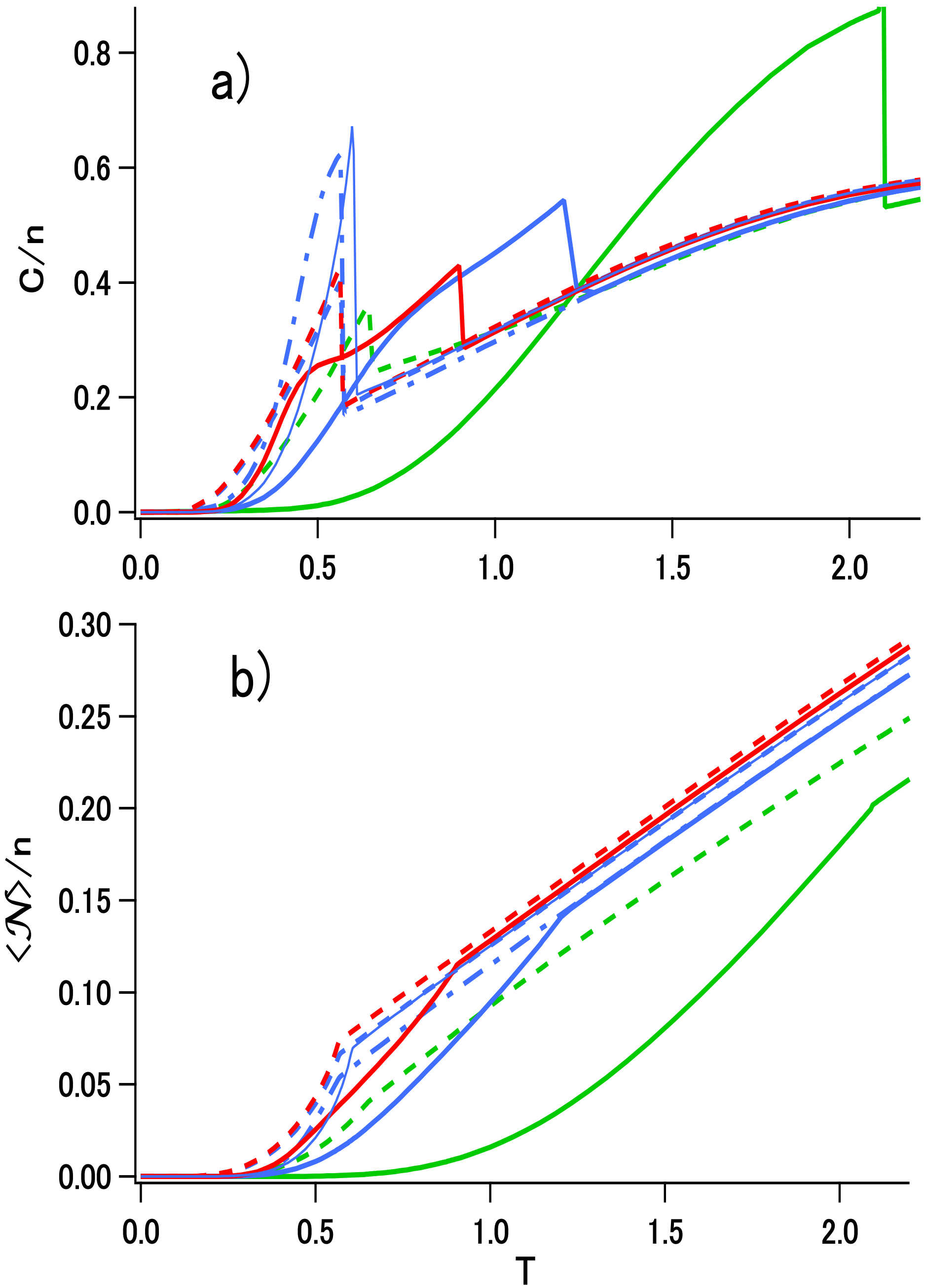
($\leftarrow$ n proj.)

$n = 10$ $\quad C_{\rm G}$: – – – – $\quad C_{\rm C}$: ——

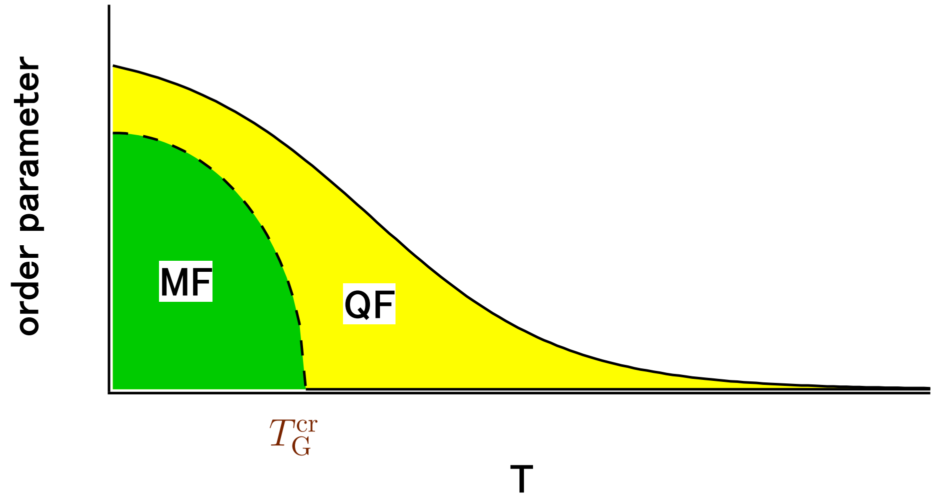
$n = 26$ $\quad C_{\rm G}$: – – – – $\quad C_{\rm C}$: ——

$\quad C_\pi$: —— $\quad C_{\rm C'}$: — · —

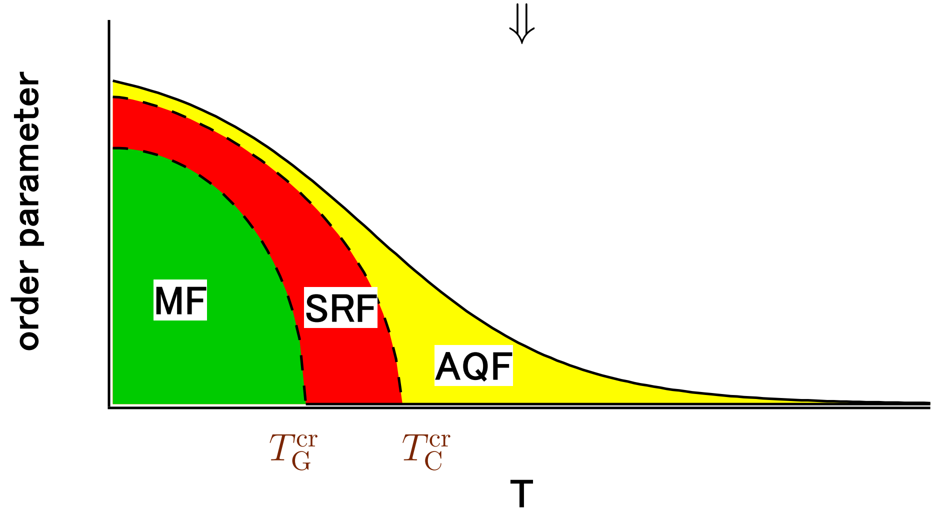
$n = 56$ $\quad C_{\rm G}$: – – – – $\quad C_{\rm C}$: ——



QF (quant. fluc.) = **SRF** (sym. restoring fluc.) + **AQF** (additional quant. fluc.)

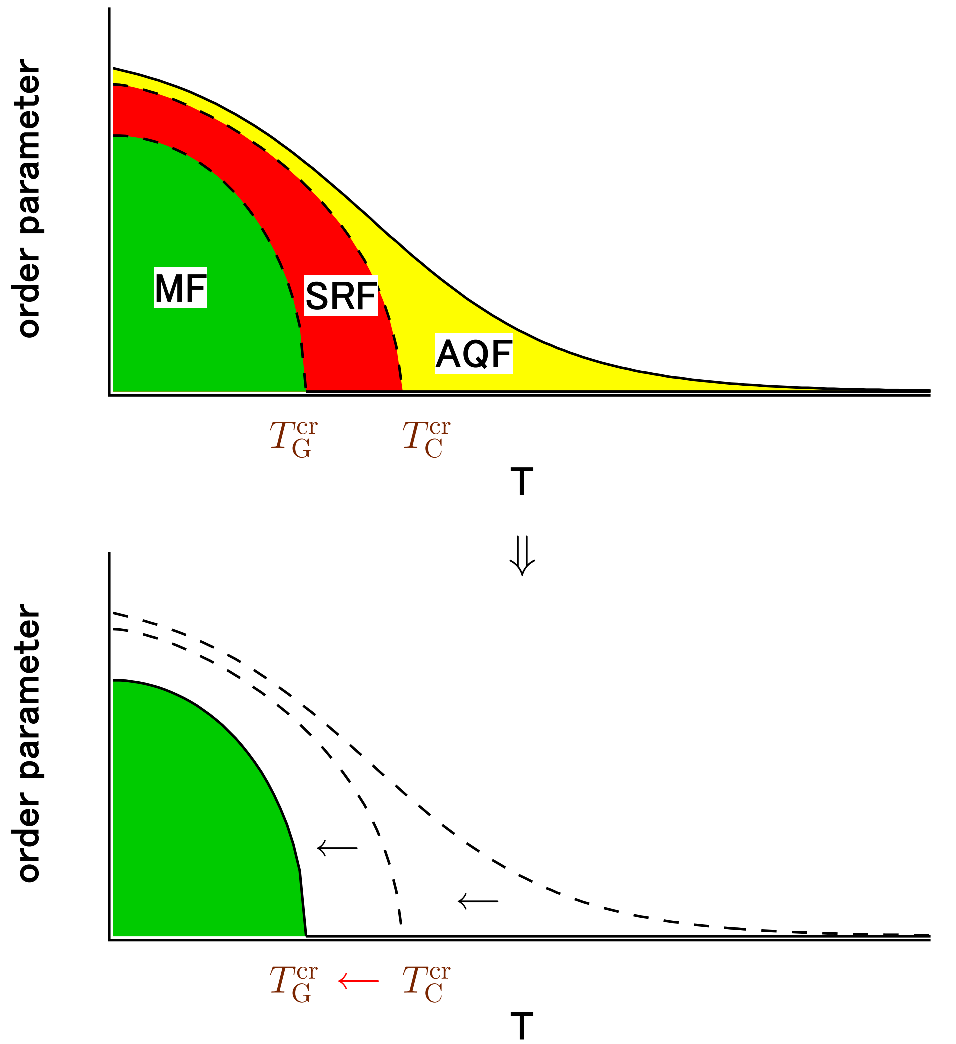


$\Downarrow$

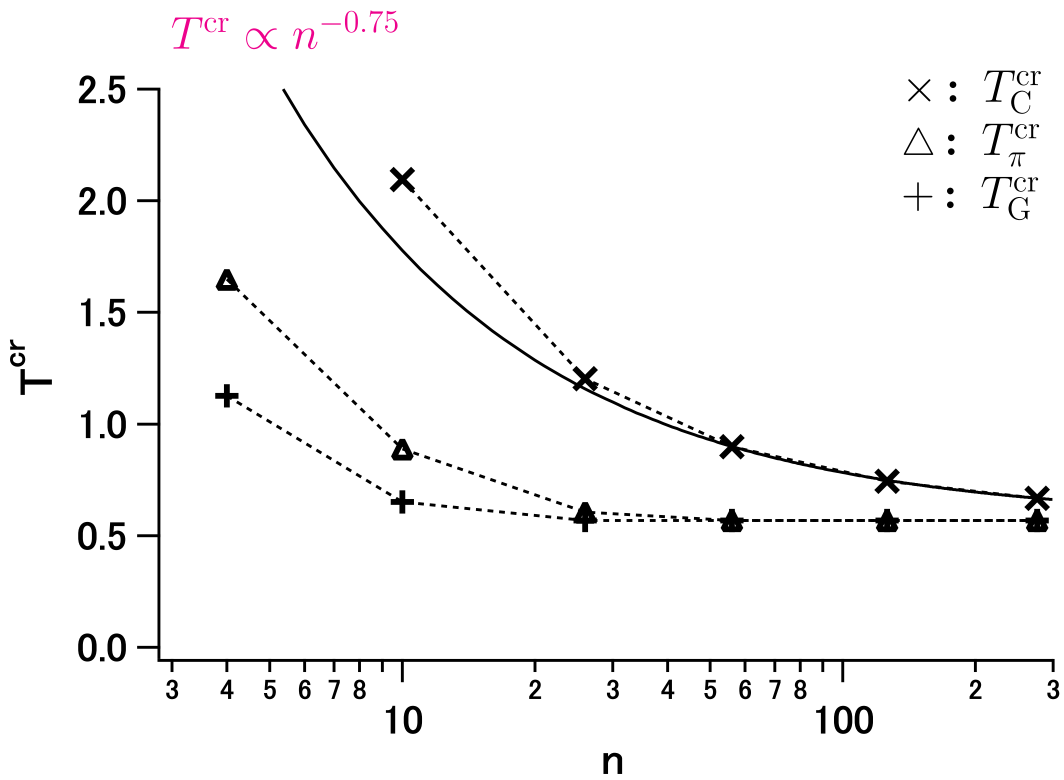


GCE-BCS (mean-field)	$\xrightarrow{}$ **SRF**	**CE-BCS** (quant. # proj.)	$\xrightarrow{}$ **AQF**	**exact**

as n grows $\cdots$



n**-dep. of** $T^{\rm cr}$ **?**



IV. Summary

1. Canonical-ensemble BCS theory is formulated for the first time.
   This theory enables us to separate the sym. restoring fluctuation (SRF)
   from the additional quantum fluctuations (AQF).

2. Via numerical studies, we find that
   the n conservation keeps the phase transition nature, but at higher $T^{\rm cr}$.

   $$\begin{cases} \text{SRF} \rightarrow \text{shifts up } T^{\rm cr} \\ \qquad \rightarrow \text{a 'phase transition' picture much closer to the reality} \\ \text{AQF} \rightarrow \text{washes out signatures of transition} \end{cases}$$

3. As n grows, both the SRF & the AQF reduce.
   The former is realized as gradual decrease of $T^{\rm cr}$.

4. These studies provide us with a new insight to phase transition in finite systems & roles of conservation laws in it.

   The effects of SRF should be taken into account
   in future investigations of 'phase transitions' in finite systems.

Ref. : H.N. & K. Tanabe, quant-ph/0603113