SCQRPA and Thermal Pairing in Nuclei

Nguyen Dinh Dang

 Nishina Center for Accelerator-Based Science, RIKEN Wako city, Saitama - Japan
 Institute for Nuclear Science & Technique Hanoi - Vietnam

Collaborator

Nguyen Quang Hung

This talk is based on

- 1. N. Quang Hung & NDD, PRC 76 (2007) 054302, 77 (2008) 029905(E)
- 2. NDD & N. Quang Hung, PRC 77 (2008) 064315
- **3**. N. Quang Hung & NDD, PRC 78 (2008) 064315
- 4. N. Quang Hung & NDD, PRC 79 (2009) 054328

(His PhD thesis, defended in November 2009)

Plan

Motivation

- 1. SCQRPA at zero T
- 2. SCQRPA at finite T
- **3.** SCQRPA at $T \neq 0$ & $M \neq 0$
- 4. Pairing gap from odd-even mass formula at $T \neq 0$
- 5. Canonical ensemble treatment of pairing within SCQRPA

Conclusions

Motivation

Infinite systems

(metal superconductors, ultra-cold gases, liquid helium, etc.)

- Superfuild-normal, liquid-gas, shape phase transitions, etc.
- Fluctuations are absent or negligible
- Described well by many-body theories such as BCS, RPA or QRPA

Finite systems

(atomic nuclei, ultra-small metallic grains, etc.)

- Phase transitions are smoothed out
- Strong quantal and thermal fluctuations
- The conventional BCS, RPA or QRPA fail in a number of cases (collapsing points, in light systems, at T≠0, at strong or weak interaction, etc.)

When applied to finite small systems, to be reliable, the BCS, RPA and/or QRPA need to be corrected to take into account the effects due to quantal and thermal fluctuations.

THE SELFCONSISTENT QRPA (SCQRPA)

Testing ground: Pairing model

$$\begin{split} H &= \sum_{j} \varepsilon_{j} \hat{N}_{j} - G \sum_{j,j^{\dagger}} \hat{P}_{j}^{\dagger} \hat{P}_{j^{\dagger}} ,\\ \hat{N}_{j} &= \sum_{m}^{\Omega_{j}} a_{jm}^{\dagger} a_{jm} , \hat{P}_{j}^{\dagger} = \frac{1}{\sqrt{\Omega_{j}}} \sum_{m=1}^{\Omega_{j}} a_{jm}^{\dagger} a_{j\tilde{m}}^{\dagger} , \hat{P}_{j} = (\hat{P}_{j}^{\dagger})^{\dagger} ,\\ \Omega_{j} &= j + \frac{1}{2} , O_{j\tilde{m}} \equiv (-)^{j-m} O_{j-m} . \end{split}$$

$$\begin{split} \left[\hat{P}_{j},\hat{P}_{k}^{+}\right] &= \delta_{jk} \left(1 - \frac{\hat{N}_{j}}{\Omega_{j}}\right), \\ \left[\hat{N}_{j},\hat{P}_{k}^{+}\right] &= 2\delta_{jk}\hat{P}_{j}^{+}, \left[\hat{N}_{j},\hat{P}_{k}\right] &= -2\delta_{jk}\hat{P}_{j}. \end{split}$$

Exact solutions: A. Volya, B.A. Brown, V. Zelevinsky, PLB 509 (2001) 37 Shortcoming: impracticable at N > 14 BCS :

Bogoliubov transformation: $a_{jm}^{+} = u_{j}\alpha_{jm}^{+} + v_{j}\alpha_{jm}^{-}, a_{jm}^{-} = u_{j}\alpha_{jm}^{-} - v_{j}\alpha_{jm}^{+}, u_{j}^{2} + v_{j}^{2} = 1,$ Qp. pair and qp. number operators: $A_{j}^{+} = \Omega_{j}^{-1/2}\sum_{m}\alpha_{jm}^{+}\alpha_{jm}^{+}, N_{j} = \sum_{m}\alpha_{jm}^{+}\alpha_{jm}^{-},$ $\begin{bmatrix} A_{j}^{-}A_{j'}^{+} \end{bmatrix} = \delta_{jj}D_{j}^{-}, D_{j}^{-} = 1 - N_{j}^{-}/\Omega_{j}^{-},$ $\begin{bmatrix} N_{j}^{-}A_{j'}^{+} \end{bmatrix} = 2\delta_{jj}A_{j}^{+}, \begin{bmatrix} N_{j}^{-}A_{j'} \end{bmatrix} = -2\delta_{jj}A_{j}^{-}.$

 $H \to H = H - \lambda N, \text{variational procedure:} \quad \langle \dots \rangle = \langle \text{BCS} | \dots | \text{BCS} \rangle, \text{ i.e. } \langle N_j \qquad \Box = 0$ $\frac{\partial \langle H \rangle}{\partial u_j} + \frac{\partial \langle H \rangle}{\partial v_j} \frac{\partial v_j}{\partial u_j} \equiv \langle [H, A_j^+] \rangle = 0,$

$$\begin{array}{l} \left(\begin{array}{c} \mathsf{QRPA} \\ \mathcal{Q}_{v}^{+} = \sum_{j} \left(X_{j}^{v} \mathsf{A}_{j}^{+} - Y_{j}^{v} \mathsf{A}_{j}^{-} \right), \ \mathcal{Q}_{v} = \left[\mathcal{Q}_{v}^{+} \right]^{+} \\ \mathcal{Q}_{v}^{+} = \left[\mathcal{Q}_{v}^{+} \right]^{+} \\ \left(\begin{array}{c} \mathsf{Quasiboson approximation (QBA):} \\ \mathsf{QBA} \end{array} \right), \ \mathcal{Q}_{v} = \left[\mathcal{Q}_{v}^{+} \right]^{+} \\ \mathcal{Q}_{v}^{-} \left[\mathsf{A}_{j}^{-} \mathsf{A}_{j}^{-} \right] \\ \mathcal{Q}_{v}^{+} \left[\mathsf{A}_{j}^{-} \mathsf{A}_{j}^{+} \right] \\ \mathcal{Q}_{v}^{+} \left[\mathsf{A}_{j}^{-} \mathsf{A}_{j}^{+} \right] \\ \mathcal{Q}_{v}^{+} \left[\mathsf{Q}_{\mu}^{-} \mathsf{Q}_{v}^{+} \right] \\ \mathcal{Q}_{v}^{+} \left[\mathsf{Q}_{\mu v}^{-} \mathsf{Q}_{v}^{+} \right] \\ \mathcal{Q}_{\mu v}^{+} \left[\mathsf{Q}_{\mu v}^{+} \mathsf{Q}_{v}^{+} \mathsf{Q}_{v}^{+} \mathsf{Q}_{v}^{+} \right] \\ \mathcal{Q}_{\mu v}^{+} \left[\mathsf{Q}_{\mu v}^$$

QRPA reduces to (pp)RPA at $G \leq G_c$



Violation of particle number \rightarrow PNF: $\delta N^2 = \langle N^2 \rangle - \langle N \rangle^2$ \rightarrow Collapse of BCS at G \leq G_c

 $\begin{array}{l} \text{Omission of QNF:} \\ \delta N \quad \Box = \langle \ N \quad \Box \quad \Box \quad - \langle N \ \rangle^2 \\ \rightarrow \text{Collapse of BCS gap at } T = T_c \end{array}$





Shortcomings of (pp)RPA and QRPA: QBA: Violation of Pauli principle → Collapse of RPA at G ≥ G_c QRPA is valid only when BCS is valid: Collapse of QRPA at G ≤ G_c



Works in this direction

These shortcomings have been partially removed by:

Pairing:

PNP (Ring, Rossignoli, Dobacewski, Egido, et al) exact a A Generate Theory of phase transition (Moretto, Goodman) SPA (Ring, Rossignoli, NDD, et al) \rightarrow macroscopic SMCC (Dean, Koonin, Alhassid et al) \rightarrow exact at high T MBCS (NDD, Zelevinsky, Arima) \rightarrow complex RPA decreases with N in half-filled cases RRPA (Hara, Rowe, Catara, Sambataro, NDD, et al) SCRPA (Dukelsky, Schuck, et al) far from exact at G

 \rightarrow deviates from exact at G>G

Creating a Dumbo

a selfconsistent approach that works for any value of
 pairing interaction G,
 temperature T,
 angular momentum M,
 particle number N

Obviously such approach should contain the RPA and QRPA as its limits.







RPA

1. SCQRPA at T = 0

BCS equations with SCQRPA corrections

$$\begin{split} \Delta_{j} &= \Delta + \underline{\delta} \Delta_{j}, \quad N = 2\sum_{j} \Omega_{j} \left[\langle \underline{\mathsf{D}}_{j} \rangle v_{k}^{2} + \frac{1}{2} \left(1 - \langle \underline{\mathsf{D}}_{j} \rangle \right) \right], \\ \Delta &= G\sum_{j} \Omega_{j} u_{j} v_{j} \langle \underline{\mathsf{D}}_{j} \rangle, \quad \delta \Delta_{j} = 2Gu_{j} v_{j} \delta \mathsf{N}_{j}^{2} / \langle \underline{\mathsf{D}}_{j} \rangle, \\ \langle \underline{\mathsf{D}}_{j} \rangle &= 1 - 2n_{j}, \quad \delta^{-2} = n_{j} (1 - n_{j}), \quad n_{j} \equiv \langle \mathbf{N}_{j} \rangle / (2\Omega_{j}). \\ u_{j}^{2} &= \frac{1}{2} \left(1 + \frac{\varepsilon_{j}' - \lambda}{E_{j}} \right) \qquad \Delta_{j} = \frac{G}{\langle \overline{\mathcal{D}}_{j} \rangle} \sum_{j'} \Omega_{j'} \langle \mathcal{D}_{j} \mathcal{D}_{j'} \rangle u_{j'} v_{j'}, \\ \varepsilon_{j}' &= \varepsilon_{j} + \langle \mathcal{D}_{j} \mathcal{D}_{j'} \rangle = \langle \mathcal{D}_{j} \rangle \langle \mathcal{D}_{j'} \rangle + \frac{\delta N_{jj'}}{\Omega_{j} \Omega_{j'}}, \\ \delta N_{jj'} &= \langle \mathcal{N}_{j} \mathcal{N}_{j'} \rangle - \langle \mathcal{N}_{j} \rangle \langle \mathcal{N}_{j'} \rangle, \\ Q_{v}^{+} &= \sum_{j} \frac{1}{\sqrt{\langle \underline{\mathsf{O}}_{j} \rangle}} \left[\mathsf{X}_{j'} \mathsf{X}_{j} + \frac{\delta N_{jj'}}{2\Omega_{j} \delta N_{j}^{2} \delta_{jj'}, \quad \delta N_{j}^{2} \equiv n_{j} (1 - n_{j}), \quad \mathsf{A}_{j}^{++} \right] \rangle = \delta_{jj'} \langle \underline{\mathsf{D}}_{j} \rangle \\ \ldots \rangle &= \langle \mathsf{SCQRPA}| \ldots |\mathsf{SCQRPA}\rangle \quad \langle \underline{\mathsf{D}}_{j} \rangle = \frac{1}{1 + \frac{2}{\Omega_{j}} \sum_{v} \langle \mathbf{Y}_{j}^{v} \rangle^{2}} \quad \cdots$$
 First time derived by by Catara, NDD, Sambator NPA 570 (1994) 1

SCQRPA at T = 0 (continued)

PNP → SCQRPA + Lipkin Nogami

Coupling to pair vibrations

Doubly-folded equidistant multilevel pairing model Ω levels, N particles



Ground-state energy

Energy of first excited state

2. SCQRPA at $T \neq 0$

FT-BCS equations with QNF Thermal average in the GCE: $\langle \mathbf{O} \rangle = Tr \mathbf{O} \mathbf{e}^{-\beta \mathbf{H}} / Tr \mathbf{e}^{-\beta \mathbf{H}}$ $\Delta_{j} = \Delta + \delta \Delta_{j}, \quad N = 2\sum_{i} \Omega_{j} \left[\left\langle \mathsf{D}_{j} \right\rangle v_{k}^{2} + \frac{1}{2} \left(1 - \left\langle \mathsf{D}_{j} \right\rangle \right) \right],$ $\Delta = G \sum_{i} \Omega_{j} u_{j} v_{j} \langle \mathsf{D}_{j} \rangle, \quad \delta \Delta_{j} = 2 G u_{j} v_{j} \delta \mathsf{N}_{j}^{2} / \langle \mathsf{D}_{j} \rangle,$ $\langle \mathsf{D}_j \rangle = 1 - 2n_j, \quad \delta \mathsf{N}_j^2 = n_j (1 - n_j).$ $\varepsilon'_{j} = \varepsilon_{j} + \frac{G}{\sqrt{\Omega_{j}}\langle \mathsf{D}_{j}\rangle} \sum_{j'} \left(u_{j'}^{2} - v_{j'}^{2} \right) \left(\langle \mathsf{A}_{j'}^{+} \mathsf{A}_{j'\neq j}^{+} \rangle + \langle \mathsf{A}_{j'}^{+} \mathsf{A}_{j'} \rangle \right).$ $\langle \mathcal{A}^{\dagger}_{i} \mathcal{A}_{i'} \rangle$

$$\begin{aligned} x_{jj'} &= \frac{\langle \mathcal{X}_{j}^{\mu} \mathcal{Y}_{j'}^{\mu}}{\sqrt{\langle \mathcal{D}_{j} \rangle \langle \mathcal{D}_{j'} \rangle}} = \sum_{\mu} \mathcal{Y}_{j}^{\mu} \mathcal{Y}_{j'}^{\mu} & \langle \mathcal{Q}_{\mu}^{\dagger} \mathcal{Q}_{\mu'}^{\dagger} \rangle \\ &+ \sum_{\mu\mu'} \left(U_{jj'}^{\mu\mu'} \langle \mathcal{Q}_{\mu}^{\dagger} \mathcal{Q}_{\mu'} \rangle + Z_{jj'}^{\mu\mu'} \langle \mathcal{Q}_{\mu}^{\dagger} \mathcal{Q}_{\mu'}^{\dagger} \rangle \right), & \langle \mathcal{Q}_{\mu}^{\dagger} \mathcal{Q}_{\mu'}^{\dagger} \rangle = -\sum_{j} \mathcal{Y}_{j}^{\mu} \mathcal{X}_{j'}^{\mu'} + \sum_{jj'} \left(U_{jj'}^{\mu\mu'} y_{jj'} - W_{jj'}^{\mu\mu'} x_{jj'} \right), \\ y_{jj'} &= \frac{\langle \mathcal{A}_{j}^{\dagger} \mathcal{A}_{j'}^{\dagger} \rangle}{\sqrt{\langle \mathcal{D}_{j} \rangle \langle \mathcal{D}_{j'} \rangle}} = \sum_{\mu} \mathcal{Y}_{j}^{\mu} \mathcal{X}_{j'}^{\mu} & U_{jj'}^{\mu\mu'} \langle \mathcal{Q}_{\mu}^{\dagger} \mathcal{Q}_{\mu'} \rangle , \\ &+ \sum_{\mu\mu'} \left(U_{jj'}^{\mu\mu'} \langle \mathcal{Q}_{\mu}^{\dagger} \mathcal{Q}_{\mu'}^{\dagger} \rangle + Z_{jj'}^{\mu\mu'} \langle \mathcal{Q}_{\mu}^{\dagger} \mathcal{Q}_{\mu'} \rangle \right), \end{aligned}$$

SCQRPA at $T \neq 0$ (continued)

Some limits:

FTBCS: $n_{j} = n_{j}^{FD} = \frac{1}{e^{\beta E_{j}} + 1}, \ \delta N_{j}^{2} = 0, \ \langle A_{j}^{+}A_{j'\neq j}^{+} \rangle = \langle A_{j}^{+}A_{j'} \rangle = 0.$ FTBCS1 $n_{j} = n_{j}^{FD} = \frac{1}{e^{\beta E_{j}} + 1}, \ \delta N_{j}^{2} \neq 0, \ \langle A_{j}^{+}A_{j'\neq j}^{+} \rangle = \langle A_{j}^{+}A_{j'} \rangle = 0.$ FTLN1 = FTBCS1 + Lipkin-Nogami PNP

Dynamic coupling to SCQRPA vibrations



$$\begin{split} M_{j}(\omega) &= \sum_{\mu} \left(V_{j}^{\mu} \right)^{2} \Bigg[\frac{\left(1 - n_{j} + v_{\mu} \right) \left(\omega - \widetilde{E}_{j} - \omega_{\mu} \right)}{\left(\omega - \widetilde{E}_{j} - \omega_{\mu} \right)^{2} + \varepsilon^{2}} + \frac{\left(n_{j} + v_{\mu} \right) \left(\omega - \widetilde{E}_{j} + \omega_{\mu} \right)}{\left(\omega - \widetilde{E}_{j} + \omega_{\mu} \right)^{2} + \varepsilon^{2}} \Bigg] , \\ V_{j}^{\mu} &= \sum_{j'} g_{j}(j') \sqrt{\langle \mathsf{D}_{j'} \rangle} \left[\mathsf{X}_{j'}^{\mu} + \mathsf{Y}_{j'}^{\mu} \right), \qquad \gamma_{j}(\omega) = -\Im n \Big[M_{j}(\omega \pm i\varepsilon) \Big]. \end{split}$$

FTBCS1(FTLN1) + SCQRPA $n_{j} = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\gamma_{j}(\omega) (e^{\beta \omega} + 1)^{-1}}{[\omega - \tilde{E}_{j} - M_{j}(\omega)]^{2} + \gamma_{j}^{2}(\omega)} d\omega$



N=50

Realistic nuclei



3. Pairing in hot rotating systems



B. Mottelson and J. Valatin, PRL 5 (1960) 511 A. Goodman, NPA 369 (1981) 365 Thermally assisted pairing correlation (pairing reentrance effect)

 $T = 0, M \neq 0$

M,

M

 Δ

 $T \neq 0, M \neq 0$

normal

superfluid

T₁

 T_2

L. G. Moretto, NPA 185 (1972) 145 R. Balian, H. Flocard, M. Vénéroni, PR 317 (1999) 251

T = 0, M = 0

Hot rotating finite systems

S. Frauendorf et al., PRB 68, (2003) 024518



FIG. 2. Canonical gap $\Delta_{can}(T,\omega)$ for even (full lines) and odd (the dashed line) particle numbers, and the mean-field gap $\Delta_{mf}(T,\omega)$ (dotted line -BCS) vs the temperature T for a spherical shell.

Temperature-induced pairing correlation

SCQRPA at T \neq 0 & M \neq 0

Pairing Hamiltonian including z-projection of total angular momentum:

$$H' = H - \lambda \hat{N} - \gamma \hat{M}, M = \sum_{k} m_{k} (a_{k+}^{+} a_{k+} - a_{k-}^{+} a_{k-})$$

Bogoliubov transformation + variational procedure:

$$\begin{split} \Delta_{k} &= \Delta + \delta \Delta_{k} , & N = 2 \sum_{k} \left[v_{k}^{2} + \frac{1}{2} (1 - 2v_{k}^{2}) (n_{k}^{+} + n_{k}^{-}) \right] \\ \Delta &= G \sum_{k} u_{k} v_{k} \langle \mathsf{D}_{k} \rangle , & \boldsymbol{\mathcal{E}} & M = \sum_{k} m_{k} (n_{k}^{+} - n_{k}^{-}) \\ \delta \Delta_{k} &= G u_{k} v_{k} \langle \mathsf{N}_{k}^{2} / \langle \mathsf{D}_{k} \rangle , & u_{k}^{2} = \frac{1}{2} \left(1 + \frac{\varepsilon_{k}' - \lambda}{E_{k}} \right) v_{k}^{2} = \frac{1}{2} \left(1 - \frac{\varepsilon_{k}' - \lambda}{E_{k}} \right) \\ \langle \mathsf{D}_{k} \rangle &= 1 - n_{k}^{+} - n_{k}^{-} , & E_{k} = \sqrt{(\varepsilon_{k}' - \lambda - Gv_{k}^{2})^{2} + \Delta_{k}^{2}} \end{split}$$

FTBCS1: $\langle A_k^{\dagger}A_{k'}^{\dagger} \rangle = \langle A_k^{\dagger}A_{k'} \rangle = 0, \quad n_k^{\pm} = \frac{1}{1 + \exp[\beta (E_k \mp \gamma m_k)]}.$

Dynamic coupling to SCQRPA vibrations (T \neq 0 & M \neq 0)

$$G_{k}^{\pm}(E) = \frac{1}{2 \pi} \frac{1}{E - \tilde{E}_{k} \mp \gamma m_{k} - M_{k}^{\pm}(E)},$$

$$\tilde{E}_{k} = b_{k}' + q_{kk},$$

$$b_{k}' = (\mathcal{E}_{k} - \lambda)(u_{k}^{2} - v_{k}^{2}) + 2 G_{k} \psi v_{k} \sum_{k'} u_{k'} v_{k'} + G_{k}^{4},$$

$$q_{kk} = -G_{k}^{2} \psi_{k}^{2}, \quad g_{k}(k') = G_{k} \psi v_{k} (u_{k'}^{2} - v_{k'}^{2}),$$

$$M_{k}^{\pm}(E) = \sum_{\mu} \left(V_{k}^{\mu} \right)^{2} \left[\frac{1 - n_{k}^{\pm} + v_{\mu}}{E - \widetilde{E}_{k} \mp \gamma m_{k} - \omega_{\mu}} + \frac{n_{k}^{\pm} + v_{\mu}}{E - \widetilde{E}_{k} \mp \gamma m_{k} + \omega_{\mu}} \right],$$
$$V_{k}^{\mu} = \sum_{k'} g_{k}(k') \sqrt{\langle \mathsf{D}_{k'} \rangle} \left[\mathsf{X}_{k'}^{\mu} + \mathsf{Y}_{k'}^{\mu} \right], \ \gamma_{k}^{\pm}(\omega) = - \Im m \left[M_{k}^{\pm}(\omega \pm i\varepsilon) \right].$$

$$n_{k}^{\pm} = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\gamma_{k}(\omega) (e^{\beta \omega} + 1)^{-1}}{[\omega - \tilde{E}_{k} \mp \gamma n_{k} - M_{k}(\omega)]^{2} + \gamma_{k}^{2}(\omega)} d\omega$$

FTBCS1:
$$n_k^{\pm} = \frac{1}{1 + \exp[\beta (E_k \mp \gamma m_k)]}, \quad \langle A_k^{\dagger} A_{k'}^{\dagger} \rangle = \langle A_k^{\dagger} A_{k'} \rangle = 0.$$











4. Odd-even mass formula at $T \neq 0$

$$\begin{split} \Delta^{(3)}(\beta,N) &\simeq \frac{(-1)^N}{2} [\langle \mathcal{E}(N+1) \rangle - 2\langle \mathcal{E}(N) \rangle + \langle \mathcal{E}(N-1) \rangle], \\ \Delta^{(4)}(\beta,N) &= \frac{1}{2} [\Delta^{(3)}(N) + \Delta^{(3)}(N-1)]. \end{split}$$
Uncorrelated s.p energy
$$\langle \mathcal{E}(N) \rangle &= \langle \mathcal{E}(N) \rangle^{(0)} - \frac{\Delta^2(\beta,N)}{G} \\ \langle \mathcal{E} \rangle^{(0)} &\equiv 2 \sum_j \Omega_j \epsilon_j f_j - G \sum_j \Omega_j f_j^2 \\ \tilde{\Delta}^{(3)}(\beta,N) &= (-1)^N \left\{ \frac{1}{2} [\langle \mathcal{E}(N+1) \rangle + \langle \mathcal{E}(N-1) \rangle] - \langle \mathcal{E} \rangle^0 + \frac{[\tilde{\Delta}^{(3)}(\beta,N)]^2}{G} \right\} \\ \tilde{\Delta}^{(3)}(\beta,N) &= \frac{G}{2} \left[(-1)^N + \sqrt{1-4\frac{S}{G}} \right] \\ S &= \frac{1}{2} [\langle \mathcal{E}(N+1) \rangle + \langle \mathcal{E}(N-1) \rangle] - \langle \mathcal{E}(N) \rangle^{(0)} \end{split}$$

Odd-even mass formula at $T \neq 0$



5. Latest development:

Current problems in the study of nuclear pairing at $T \neq 0$

Exact solutions

- Impracticable at N > 14 (for N= Ω =16 : 5,196,627 states, i.e. a square matrix of order ~ 2.7 x 10¹³)
- Differences between the predictions within GCE, CE and MCE in small systems
- Ambiguity in the temperature extracted from MCE (negative temperatures)

Theoretical approximations

- Derived within the GCE
- Results are compared with exact solutions in CE
- Workable for wide range of mass
- Differences between theoretical (GCE) and exact CE pairing gap at high T

Because N is fixed, CE should be used in application to nuclei

It is therefore desirable to construct an approach based on the CE, which offers results in good agreement with the exact CE ones for any (or at least larger) values of N.

Method: Embedding the eigenvalues at T=0 in the CE

Partition function:
$$Z(\beta) = \sum_{s=0,2,4}^{\Omega} d_s e^{-\beta E_s}$$
, Total energy $\langle \mathsf{E} \rangle = -\frac{\partial \ln Z(\beta)}{\partial \beta} = Z(\beta)^{-1} \sum_s d_s E_s e^{-\beta E_s}$
Heat capacity $C = \frac{\partial \langle \mathsf{E} \rangle}{\partial T}$, Pairing gap $\Delta = \sqrt{-G(\langle \mathsf{E} \rangle - 2\sum_j \Omega_j \varepsilon_j f_j + G\sum_j \Omega_j f_j^2)}$
CE-BCS
Gap and number equations at T=0: $\Delta = G\sum_j \Omega_j u_j v_j$, $N = 2\sum_j \Omega_j v_j^2$.
Ground-state energy (at T=0): $\mathsf{E}_s^{BCS} = 2\sum_j \Omega_j \varepsilon_j v_j^2 - G^{-1} \Delta^2 - G\sum_j \Omega_j v_j^4$
Solve BCS equations for each set of total seniority S to get Δ_S^{BCS} , E_S^{BCS}
CE partition function, energy and pairing gap $Z_{CE-BCS}(\beta) = \sum_s 2^S e^{-\beta \mathsf{E}_s^{BCS}}$
 $\langle \mathsf{E}(\beta) \rangle = \frac{1}{Z} \sum_s 2^S \mathsf{E}_s^{BCS} e^{-\beta \mathsf{E}_s^{BCS}} \langle \Delta(\beta) \rangle = \frac{1}{Z} \sum_s 2^S \Delta_S^{BCS} e^{-\beta \mathsf{E}_s^{BCS}}$

CE-LNQRPA = CE-BCS (QRPA) + LN particle number projection CE-SCQRPA = CE-LNQRPA + ground-state correlations

Numbers of eigenstates for $N = \Omega = 10$

S	Exact	CE-(LN)BCS	CE-(LN)QRPA (excluding spurious)
0	$C_5^{10} = 252$	1	10
2	$C_2^{10} C_4^{8} = 3150$	45	360
4	$\sum_{c=10}^{10} \sum_{s=0}^{0} \sum_{s=0}^{10} \frac{2}{s} \sum_{s=0}^{10} \frac{1}{s} \sum_$	$\sum_{k=0}^{2} C_{0s}^{\Omega}$	$\sum_{s} C_{s}^{\Omega} (\Omega - S)$
6	$C_{36} C_{2} = p_1 \ge 0 q_2$ $C_{10} C_{12} = 90$	45	s 90
8	1	1	1
€10	8953€	512 €	2561
Total	n _{ce-bcs(QRPA)} / n _{ex}	act decreases as	N increases.

Computing time

Ν	Exact	SQMC (estimated)	Present approach
10	1 hour	1 hour	1 second
12	10 hours	10 hours	10 seconds
14	1 day	1 day	1 minute
16	impossible	3 days	10 minutes
28	impossible	10 days	1 day

$N = \Omega = 10 \sim 14$, G = 1 MeV





Conclusions

- A microscopic selfconsistent approach to pairing called the SCQRPA is developed. It includes the effects of QNF and dynamic coupling to pair vibrations.
- Microscopic confirmation: Because of QNF, the sharp SN phase transition is smoothed out in finite systems, and a tiny rotating system in the normal state (at M > M_c and T=0) can turn superconducting at T≠0.
- The SCQRPA with LN PNP works for any values of G, N, T and M, even at large N, where the exact solutions are impracticable because of the huge size of the matrix to be diagonalized.
- A modified formula is suggested for extracting the pairing gap from the differences of total energies of odd and even systems at T≠0. By subtracting the uncorrelated single-particle motion, the new formula produces a pairing gap in reasonable agreement with the exact results.
- A novel approach called CE-LNSCQRPA is proposed, which embeds the LNSCQRPA eigenvalues into the CE, and gives results very close to exact solutions as well as the FTQMC ones. It is simple and workable for a wider range of mass (N ≤28), where the exact solution is impracticable and/or the FTQMC are time consuming. At N > 28 large HD and memory are required (for N = Ω = 28, CE-BCS (CE-LNBCS): 10⁹ eigenstates → 10 Gb of data file; CE-QRPA (CE-LNSQRPA): ~ 10¹¹ eigenstates → 100 Gb of data file.