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Thermodynamic limit and order parameter of the reduced BCS Hamiltonian

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BCS theory, a central paradigm

Superconductivity

Atomic nuclei

Superfluid ^{3}He

Color superconductivity

Ultracold fermionic gases

Topological superconductivity

BCS theory – a Hamiltonian and an ansatz[a]

Reduced BCS Hamiltonian:

$$H = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \frac{g}{V} \sum_{\mathbf{k},\mathbf{k}'} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}, \qquad g > 0.$$

BCS ansatz for the ground state:

$$|\Psi_0^{\mathrm{BCS}}\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} \right) |0\rangle, \qquad u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1.$$

The variational parameters $u_{\mathbf{k}}$, $v_{\mathbf{k}}$ are related to the gap parameter Δ, which is determined by minimizing the expectation value $\langle \Psi_0^{\mathrm{BCS}} | (H - \mu N) | \Psi_0^{\mathrm{BCS}} \rangle$, where N is the number of electrons and μ is the chemical potential.

[a] J. Bardeen, L. N. Cooper and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

Fixed μ versus fixed N

The BCS ground state with fixed μ does not conserve the number of electrons and thus contradicts the superselection rule for the total charge. In the BCS paper it was argued that in the thermodynamic limit the number fluctuations die out. Therefore one may ignore the issue of exact number conservation.

For systems with a moderate number of particles, such as atomic nuclei or ultrasmall metallic grains, a BCS state projected onto the subspace with N particles is often used. In this case the expectation value of the pair operator, the usual order parameter, vanishes and one has to look for alternatives, for instance the concept of off-diagonal long-range order[a].

[a] C. N. Yang, Rev. Mod. Phys. **34**, 694 (1962).

Exact in the thermodynamic limit? Early answers:

"It is possible that Ψ_0 is exact in the statistical limit."[a]

"We expect the quantum fluctuations to average out" and corrections to BCS theory to produce at most $1/N$ effects.[b]

The BCS free energy is exact in this limit.[c,d]

"The trial function ... does asymptotically, and on the average, approach the exact eigenfunction of the problem."[e]

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[a] BCS paper (1957)
[b] P. W. Anderson, Phys. Rev. **112**, 1905 (1958)
[c] N.N. Bogoliubov *et al.*, Sov. Phys. JETP **12**, 88 (1961)
[d] B. Mühlschlegel, J. Math. Phys. **3**, 522 (1962)
[e] D. C. Mattis and E. H. Lieb, J. Math. Phys. **2**, 602 (1961)

Our comparison between the exact and BCS ground states[a]

For certain quantities – ground state energy, order parameter, pseudospin-pseudospin correlation function – BCS theory is exact in the thermodynamic limit.

For some more subtle quantities – non-diagonal pair-pair correlation function, fidelity susceptibility – the large system limit of the exact solution differs from the mean-field solution of BCS.

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[a] O. El Araby and D. Baeriswyl, Phys. Rev. B **89**, 134521 (2014).

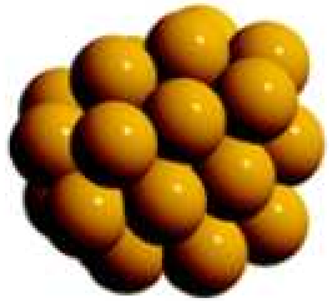
Outline

1. Richardson model and its exact solution
2. Numerical algorithm and ground state energy
3. Order parameter and off-diagonal long-range order (ODLRO)
4. Correlation functions
5. Fidelity susceptibility
6. Summary and outlook

1. Richardson model and its exact solution

Cooper pairing in finite-size systems

Fundamental question:	Anderson 1959
Nuclei:	Bohr, Mottelson and Pines 1958
Granular films:	Zeller and Giaever 1969
Nanosize Al particles:	Tinkham 1995-1997



Richardson model

$$H = \sum_{\nu\sigma} \varepsilon_\nu c^\dagger_{\nu\sigma} c_{\nu\sigma} - \frac{g}{L} \sum_{\nu,\nu'} c^\dagger_{\nu\uparrow} c^\dagger_{\nu\downarrow} c_{\nu'\downarrow} c_{\nu'\uparrow}$$

– $c^\dagger_{\nu\sigma}$, $c_{\nu\sigma}$ fermionic creation and annihilation operators

– Spectrum: $\varepsilon_\nu = -\frac{W}{2} + \frac{W}{L}(\nu - \frac{1}{2})$, $\nu = 1, ..., L$; non-degenerate, electron-hole symmetric, bandwidth W (which will be used as unit of energy, i.e. $W = 1$).

– Exact eigenstates found by Richardson[a b c]

[a] R. W. Richardson, Phys. Lett. **3**, 277 (1963)
[b] R. W. Richardson and N. Sherman, Nucl. Phys. **52**, 221 (1964)
[c] R. W. Richardson, J. Math. Phys. **6**, 1034 (1965)

BCS approximation

$$|\Psi_0^{\mathrm{BCS}}\rangle = \prod_\nu (u_\nu + v_\nu c^\dagger_{\nu\uparrow} c^\dagger_{\nu\downarrow})|0\rangle \propto e^{B^\dagger}|0\rangle\,, \quad B^\dagger = \sum_\nu \frac{v_\nu}{u_\nu} c^\dagger_{\nu\uparrow} c^\dagger_{\nu\downarrow}\,.$$

The coefficients u_ν and v_ν depend in the usual way on the gap parameter Δ, which vanishes for $g < g_c(L)$ and is finite for $g > g_c(L)$.

Thermodynamic limit (for an average number of electrons $\langle N\rangle = L$):

$$\begin{aligned} g_c(L) &\approx [\log(2L) + \gamma]^{-1} \to 0, \\ \Delta &\to \left(2\sinh\frac{1}{g}\right)^{-1}, \quad E_0 \to -\frac{L}{4}\coth\frac{1}{g}\,. \end{aligned}$$

Projection of $|\Psi_0^{\mathrm{BCS}}\rangle$ onto a definite number of $N = 2M$ electrons:

$$|\Psi_0^{\mathrm{BCS(N)}}\rangle \propto (B^\dagger)^M|0\rangle\,.$$

Exact eigenstates

Singly-occupied and doubly-occupied levels are decoupled. In the ground state no level is singly occupied and we can write the Hamiltonian as

$$H = \sum_{\nu=1}^{L} 2\varepsilon_\nu b_\nu^\dagger b_\nu - \frac{g}{L} \sum_{\nu,\nu'} b_\nu^\dagger b_{\nu'} \,, \quad b_\nu^\dagger = c_{\nu\uparrow}^\dagger c_{\nu\downarrow}^\dagger \,.$$

Eigenstates for $N = 2M$ electrons:

$$|\Psi\rangle = \prod_{i=1}^{M} B_i^\dagger |0\rangle \,, \quad B_i^\dagger = \sum_{\nu=1}^{L} \frac{1}{2\varepsilon_\nu - E_i} b_\nu^\dagger \,,$$

where the parameters E_i, $i = 1, ..., M$, are solutions of Richardson's equations

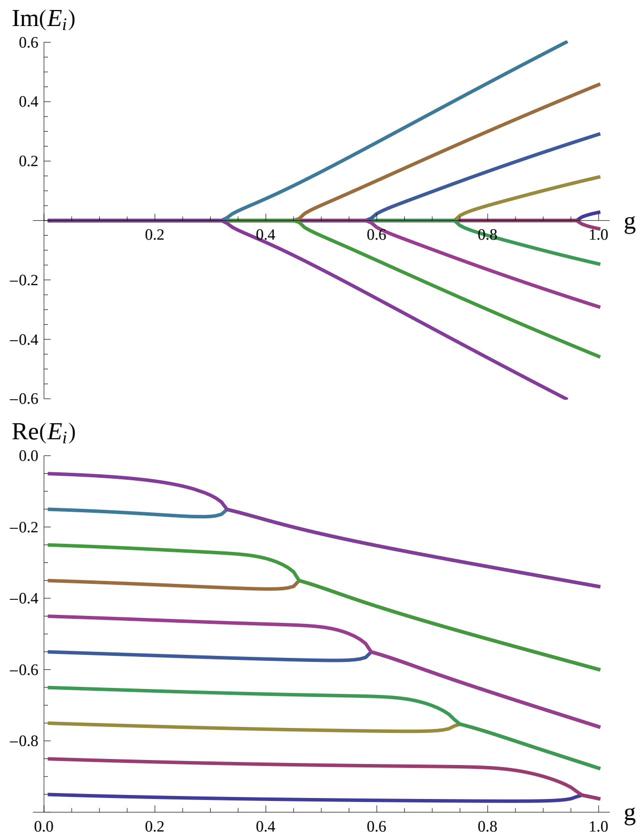
$$\frac{L}{g} - \sum_{\nu=1}^{L} \frac{1}{2\varepsilon_\nu - E_i} + \sum_{j=1 (j\neq i)}^{M} \frac{2}{E_j - E_i} = 0 \,.$$

Total energy: $E = \sum_{i=1}^{M} E_i$.

Parameters E_i ("rapidities")

The parameters E_i turn out to be complex for large enough couplings. To which extent the threshold values of g coincide with an "onset of superconductivity" remains to be clarified.

The figure shows numerical results for a spectrum of equally spaced levels (Richardson model), with $L = N = 20$.



2. Numerical algorithm and ground state energy

Numerical approach

A recently introduced algorithm uses the variables

$$\Lambda(\varepsilon_\nu) = \frac{g}{L} \sum_{i=1}^{M} \frac{1}{2\varepsilon_\nu - E_i},$$

which satisfy the "substituted Bethe equations"[a]

$$\Lambda^2(\varepsilon_\nu) - \Lambda(\varepsilon_\nu) - \frac{g}{2L} \sum_{\mu,\mu\neq\nu} \frac{\Lambda(\varepsilon_\mu) - \Lambda(\varepsilon_\nu)}{\varepsilon_\mu - \varepsilon_\nu} = 0.$$

These equations are much easier to solve than the original Richardson equations. Some quantities can be directly expressed in terms of these variables and may therefore be evaluated for very large system sizes. For other quantities one may still calculate first these variables, from which the rapidities can be extracted.[b]

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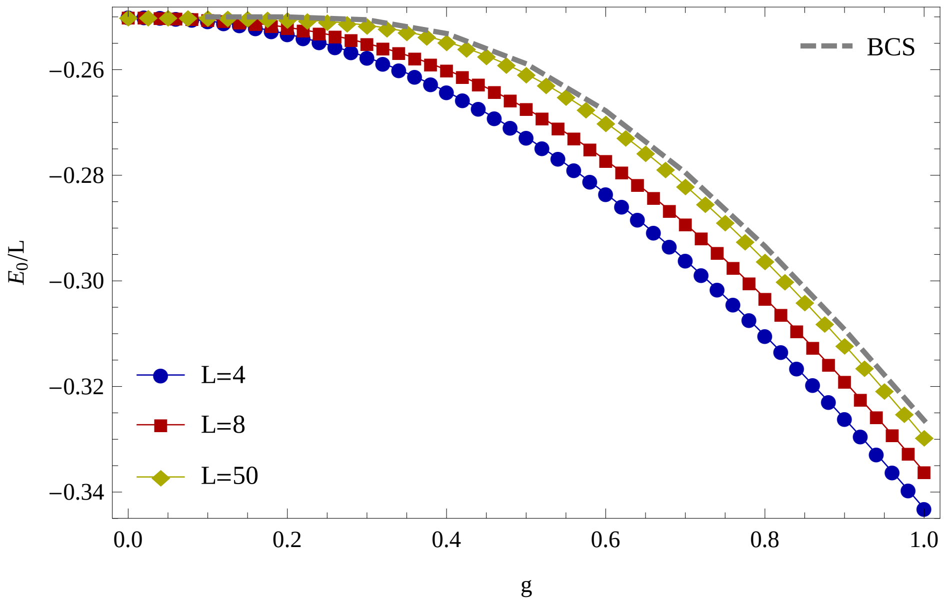
[a] A. Faribault, O. El Araby, C. Sträter and V. Gritsev, Phys. Rev. B **83**, 235124 (2011).
[b] O. El Araby, V. Gritsev and A. Faribault, Phys. Rev. B **85**, 115130 (2012).

Ground-state energy E_0

Half-filled band ($L = N$):

$$E_0 = 2\sum_{\nu} \varepsilon_{\nu}\Lambda(\varepsilon_{\nu}) - \frac{Lg}{4}.$$



The results show clearly that the exact values of the ground-state energy tend rapidly towards the asymptotic ($L \to \infty$) BCS result.

3. Order parameter and off-diagonal long-range order

Superconducting order parameter

In conventional BCS theory (fixed chemical potential) the order parameter is defined as[a]

$$F = \sum_\nu \langle \Psi_0 | b_\nu^\dagger | \Psi_0 \rangle$$

and amounts to $L\Delta/g$. This definition is not appropriate for a fixed number of particles, where F vanishes identically. A "canonical" order parameter has been proposed *ad hoc* as an alternative by von Delft and Ralph[b], it is defined as

$$\Psi_{\mathrm{can}} = \sum_\nu \left(\langle b_\nu^\dagger b_\nu \rangle - \langle c_{\nu\uparrow}^\dagger c_{\nu\uparrow} \rangle \langle c_{\nu\downarrow}^\dagger c_{\nu\downarrow} \rangle \right) .$$

We have realized that this quantity is in full agreement with Yang's concept of ODLRO.

[a] L. P. Gor'kov, JETP **9**, 1364 (1959).

[b] J. von Delft and D. C. Ralph, Phys. Rep. **345**, 61 (2001).

Off-diagonal long-range order

According to Yang[a] ODLRO exists if and only if the largest eigenvalue ω_{max} of the reduced density matrix C with matrix elements

$$C_{\mu,\nu} = \langle \Psi_0 | b_\mu^\dagger b_\nu | \Psi_0 \rangle$$

is of the order of the number of particles (or L in the case of a fixed finite particle density).

Within BCS theory we have found that ω_{max} is equal to the canonical order parameter for $L \to \infty$ (and $\langle N \rangle = L$),

$$\omega_{\mathrm{max}}^{\mathrm{BCS}} = \frac{1}{4} \sum_\nu \frac{\Delta^2}{\varepsilon_\nu^2 + \Delta^2} = \Psi_{\mathrm{can}}^{\mathrm{BCS}} \, .$$

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[a] C. N. Yang, Rev. Mod. Phys. **34**, 694 (1962).

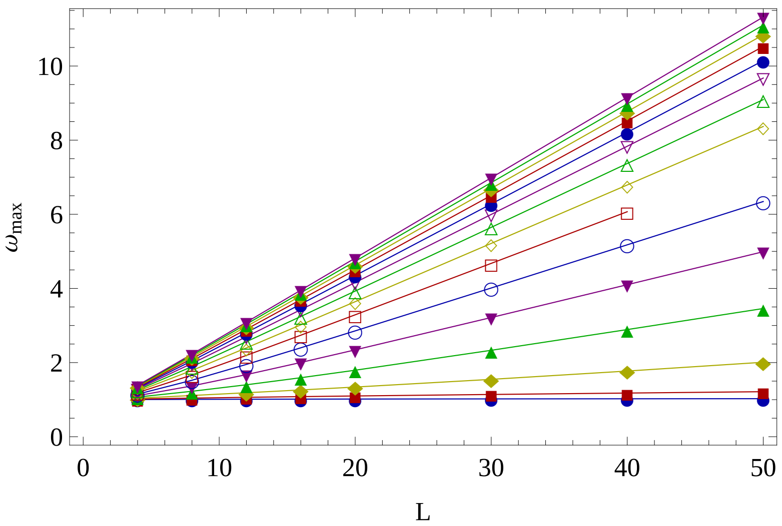
Largest eigenvalue of $C_{\mu\nu}$ within BCS theory

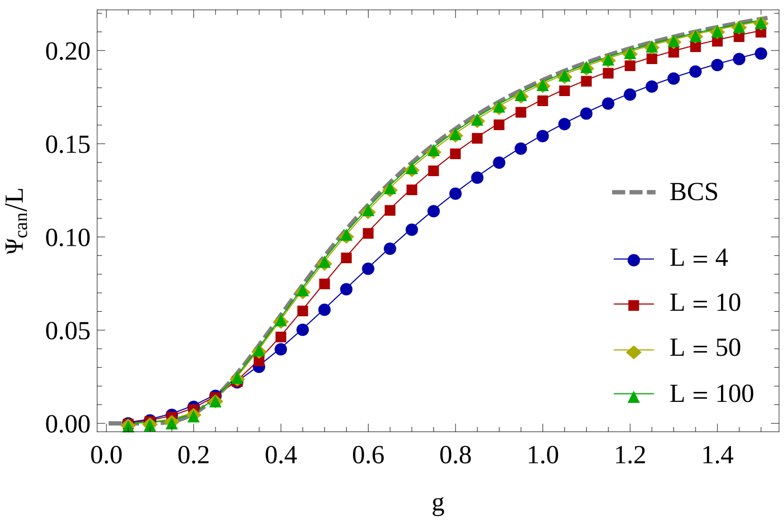
$$C_{\mu\nu}^{(\mathrm{BCS})} = \delta_{\mu\nu} \frac{(E_\nu + \varepsilon_\nu)^2}{4E_\nu^2} + \frac{\Delta^2}{4E_\mu E_\nu}\,, \qquad E_\nu := \sqrt{\varepsilon_\nu^2 + \Delta^2}\,.$$

$$\text{Eigenvalues } \omega: \qquad 1 + \sum_\nu \frac{\Delta^2}{2(\varepsilon_\nu^2 + E_\nu \varepsilon_\nu - 2E_\nu^2 \omega)} = 0\,.$$

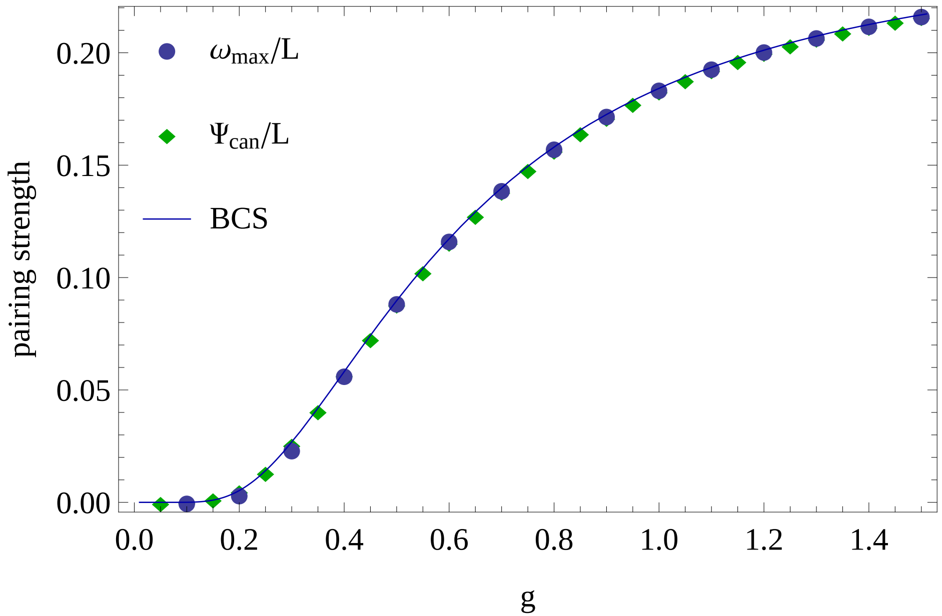
$$\text{Largest eigenvalue: } \omega_{\max}^{(\mathrm{BCS})} = \sum_\nu \frac{\Delta^2}{4E_\nu^2} \text{ for } L \to \infty.$$

Exact results for $\omega_{\max}$ and Ψ_{can}





Equivalence of ODLRO and canonical order parameter



The exact results for the largest eigenvalue agree with those for the canonical order parameter as well as with the corresponding asymptotic BCS values.

4. Correlation functions

Pseudospin-pseudospin correlation function

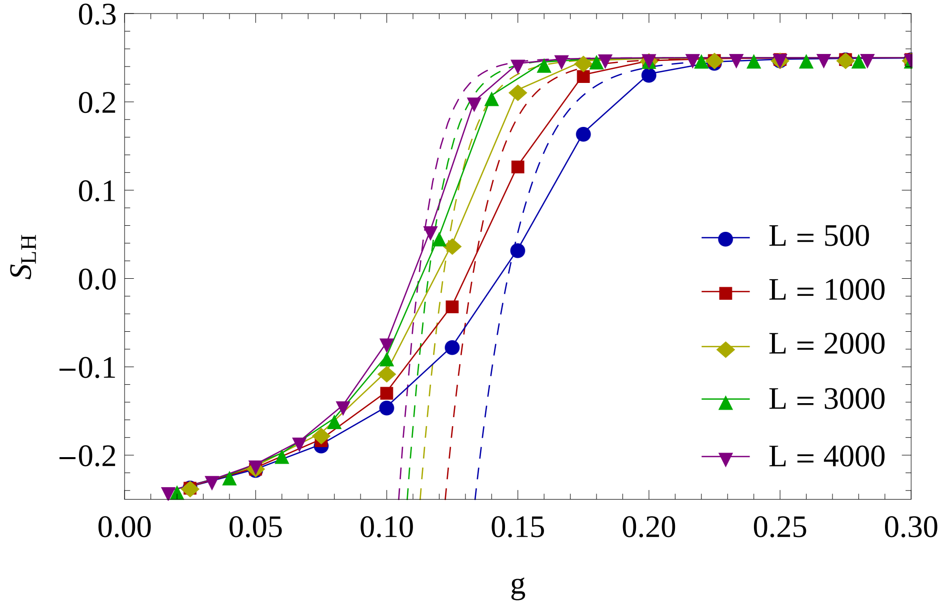
Pseudospin representation:

$$
\begin{aligned}
s_{\nu x} &= \frac{1}{2}(b_\nu + b_\nu^\dagger) \\
s_{\nu y} &= \frac{i}{2}(b_\nu - b_\nu^\dagger) \\
s_{\nu z} &= \frac{1}{2}(n_\nu - 1)
\end{aligned}
$$

$$
\begin{aligned}
H &= 2\sum_\nu \varepsilon_\nu s_{\nu z} \\
&- \frac{g}{L}\sum_{\mu,\nu,\mu\neq\nu} s_{\mu+} s_{\nu-}
\end{aligned}
$$

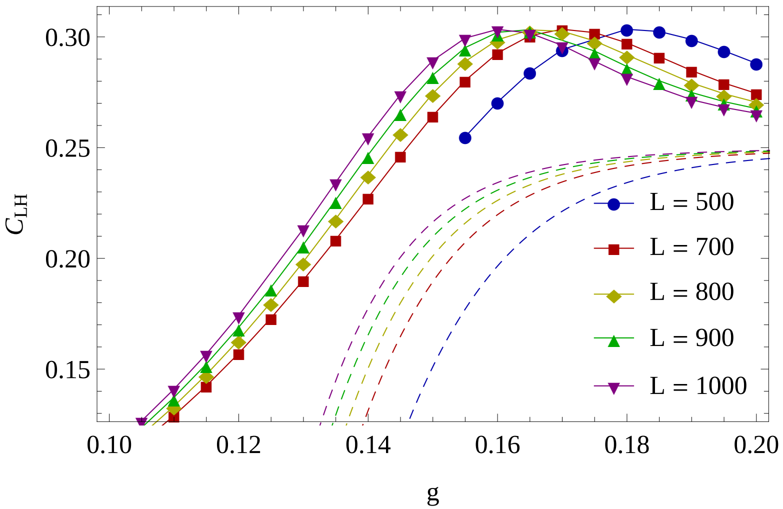
Correlation function:

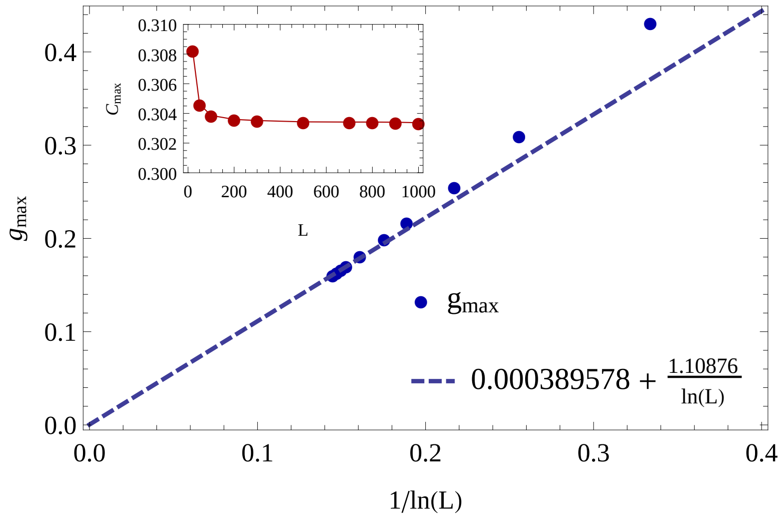
$$
S_{\mu\nu} = \langle \Psi_0 | \mathbf{s}_\mu \cdot \mathbf{s}_\nu | \Psi_0 \rangle
$$



Pair-pair correlation function

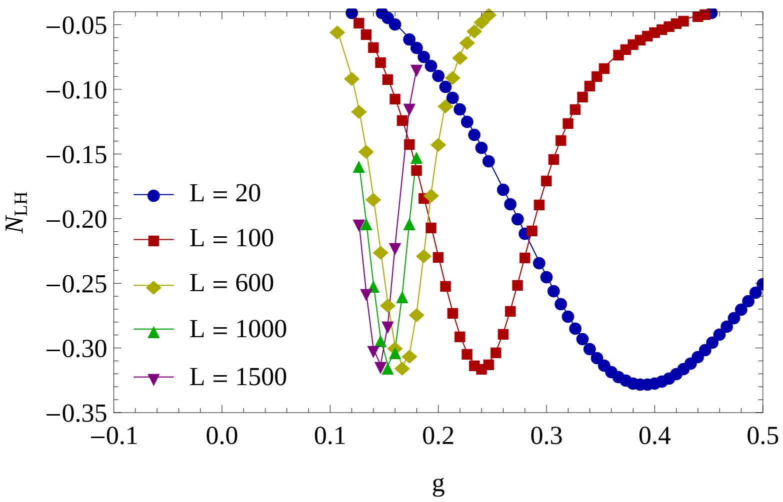
$$C_{\mu\nu} = \langle \Psi_0 | b^\dagger_\mu b_\nu | \Psi_0 \rangle = S_{\mu\nu} - \langle \Psi_0 | s_{\mu z} s_{\nu z} | \Psi_0 \rangle$$

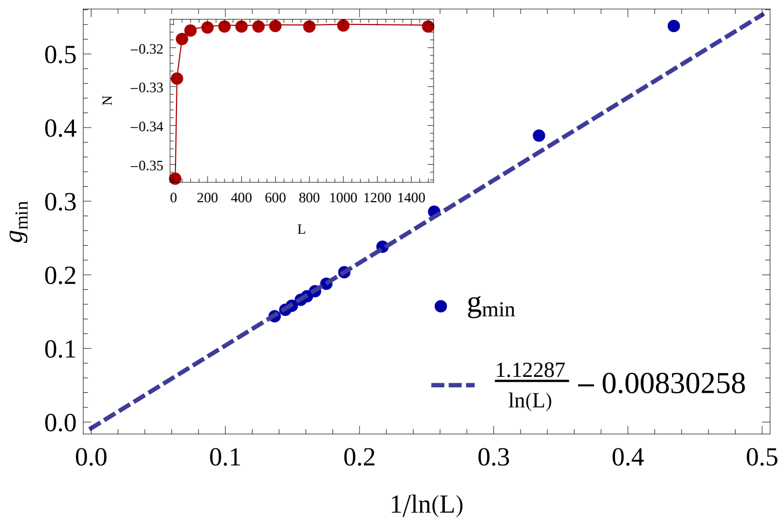




Occupancy fluctuations

$$N_{\mu\nu} = \langle \Psi_0 | (n_\mu - \langle n_\mu \rangle)(n_\nu - \langle n_\nu \rangle) | \Psi_0 \rangle$$



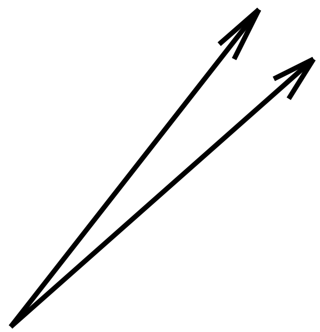


5. Fidelity susceptibility

Concept

Ground state fidelity:

$$F(g, g') = \langle \Psi_0(g) | \Psi_0(g') \rangle$$



Fidelity susceptibility[a]:

$$\chi_F(g) := -\frac{2}{L} \lim_{\delta g \to 0} \frac{\log F(g, g + \delta g)}{(\delta g)^2}$$

$$= \frac{1}{L} \sum_{n \neq 0} \sum_{\mu, \nu, \mu \neq \nu} \frac{|\langle \Psi_0(g) | b_\mu^\dagger b_\nu | \Psi_n(g) \rangle|^2}{|E_0(g) - E_n(g)|^2}$$

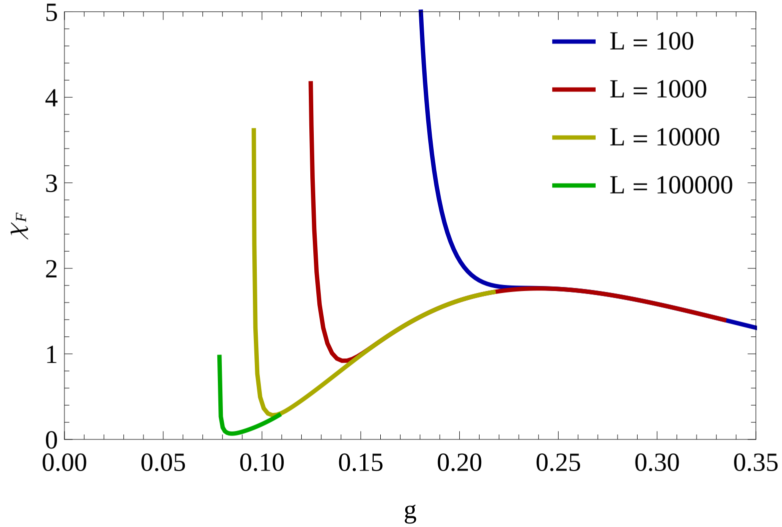
[a] P. Zanardi and N. Paunković, Phys. Rev. E **74**, 031123 (2006)

Fidelity susceptibility in BCS approximation

$$\chi_F(g) = \left(\frac{d\Delta}{dg}\right)^2 \frac{1}{4L} \sum_\nu \frac{\varepsilon_\nu^2}{(\varepsilon_\nu^2 + \Delta^2)^2}$$

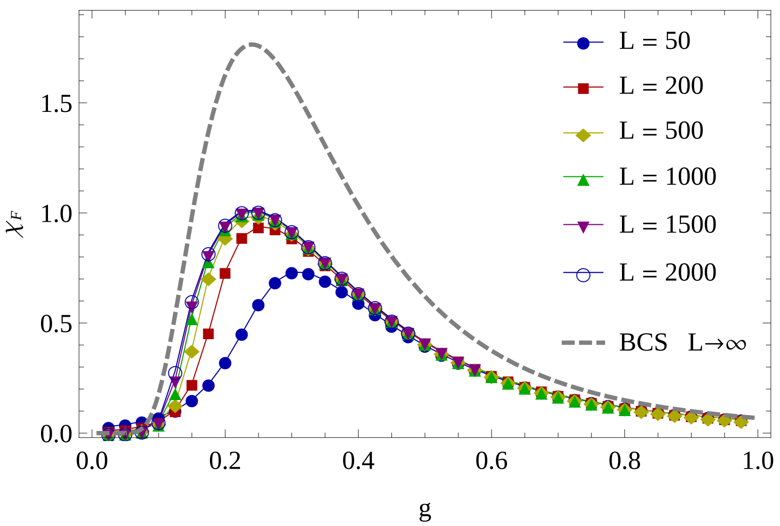
$$\to \frac{\Delta}{4g^2}\left[(1+4\Delta^2)\arctan\frac{1}{2\Delta} - 2\Delta\right]$$

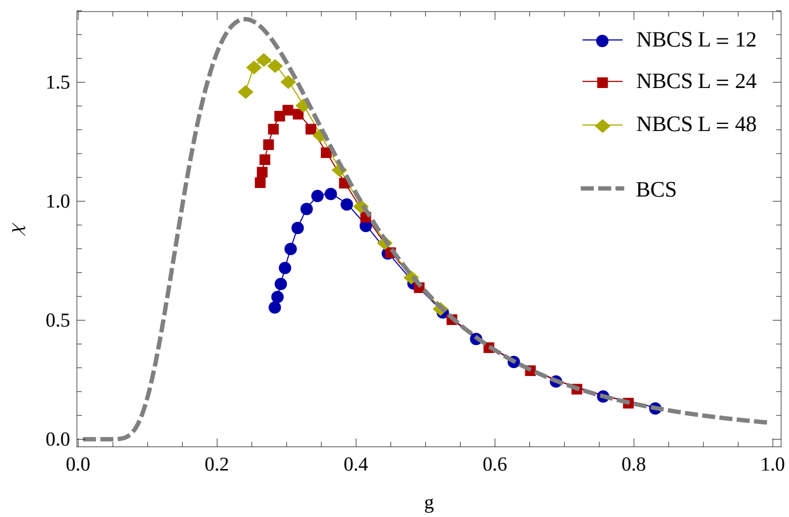
$$\text{for } L \to \infty.$$



Exact results

Number-projected BCS





Number-projected BCS state

The BCS pair operator

$$B^{\dagger} = \sum_{\nu} \left(\frac{E_{\nu} - \varepsilon_{\nu}}{E_{\nu} + \varepsilon_{\nu}} \right)^{\frac{1}{2}} b_{\nu}^{\dagger}$$

generates the number-projected BCS ground state

$$|\Psi^{(M)}\rangle = (B^{\dagger})^{M} |0\rangle$$

for M pairs. The fidelity is given by

$$F(g, g') = \frac{V^{(M)}}{\sqrt{Z(M) Z'(M)}} \,,$$

where

$$V(M) := \langle \Psi_m^{(M)} | \Psi_m^{'(M)} \rangle \,, \quad Z(M) := \langle \Psi_m^{(M)} | \Psi_m^{(M)} \rangle$$

and $|\Psi^{'(M)}\rangle$ is the ground state for the coupling strength g'.

Recursive method

The action of the operator b_ν on $|\Psi^{(M)}\rangle$ is given by

$$b_\nu|\Psi^{(M)}\rangle = M f_\nu |\Psi^{(M-1)}\rangle - M(M-1) f_\nu^2 b_\nu^\dagger |\Psi^{(M-2)}\rangle \,,$$

where $f_\nu := \Delta/(2E_\nu)$, leading to a recursion relation for the norm

$$Z^{(M)} = M Z^{(M-1)} \sum_\nu f_\nu^2 - M(M-1) \sum_\nu f_\nu^3 S_\nu^{(M-1)} \,,$$

where

$$S_\nu^{(M)} := \langle \Psi^{(M)} | b_\nu^\dagger | \Psi^{(M-1)} \rangle$$

is calculated through

$$S_\nu^{(M)} = M f_\nu Z^{(M-1)} - M(M-1) f_\nu^2 S_\nu^{(M-1)} \,.$$

6. Summary and outlook

Many quantities, such as the ground-state energy and the pseudospin-pseudospin correlation function, are predicted correctly by BCS theory in the thermodynamic limit.

Yang's concept of ODLRO is encoded in a "canonical" order parameter.

Some non-diagonal (with respect to level indices μ, ν) correlation functions and the fidelity susceptibility are not reproduced exactly by BCS theory.

We conclude that the BCS state is not the exact ground state of the reduced BCS Hamiltonian in the thermodynamic limit.

The main difference between the exact ground state and BCS is the quantum-critical behavior, where fluctuations beyond BCS produce non-perturbative corrections.

Outlook

It would be worthwhile to study the problem of the thermodynamic limit in more depth, by investigating other aspects or models:

Dynamics

Other integrable models (such as $p + ip$ pairing)

Models leading to gap parameters with zeroes (p-wave, d-wave)

Field theory