Superconductivity in small grains: Ground state thermodynamic limit and excitations

J.M. Román and G. Sierra IFT – CSIC/UAM

J. Dukelsky IEM – CSIC

Nucl. Phys. B 634 (2002) 483.

Outline:

1. Introduction: Reduced BCS Hamiltonian
2. Richardson equations
3. Integrability of the BCS Hamiltonian
4. Continuum limit: BCS equations
5. Numerical results
   - 5.1. Two-level model
   - 5.2. Equally spaced model
6. Excitations: Pics
7. Conclusions and prospects

1. Introduction: Reduced BCS Hamiltonian

The Hamiltonian for the study of a superconducting system with *N*-levels is given by:

$$H = \sum_{i=1}^{N} \sum_{\sigma=\uparrow,\downarrow} \frac{\varepsilon_{i,\sigma}}{2} c^{\dagger}_{i,\sigma} c_{i,\sigma} - \sum_{i,j=1}^{N} G_{ij} c^{\dagger}_{i,\uparrow} c^{\dagger}_{i,\downarrow} c_{j,\downarrow} c_{j,\uparrow}$$

$\varepsilon_{i,\sigma} \rightarrow \varepsilon_i$ (no spin dependence)

$G_{ij} \rightarrow G$ (reduced coupling)

$$\left.\begin{aligned} b^{\dagger}_i &= c^{\dagger}_{i,\uparrow} c^{\dagger}_{i,\downarrow} \\ b_i &= c_{i,\downarrow} c_{i,\uparrow} \end{aligned}\right\}$$

PAIR OPERATORS

$$\left.\begin{aligned} [b_i, b^{\dagger}_j] &= \delta_{ij}(1 - b^{\dagger}_i b_j) \\ b_i^2 &= (b^{\dagger}_i)^2 = 0 \end{aligned}\right\}$$

Hard-core bosons

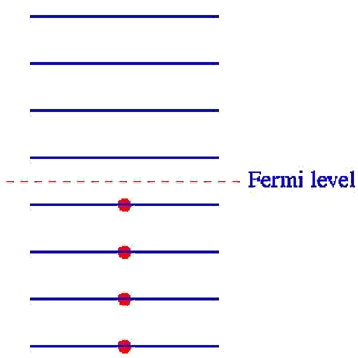
We can rewrite the one-body term:

$$c^{\dagger}_{i,\uparrow} c_{i,\uparrow} = b^{\dagger}_i b_i + n_{i,\uparrow}(1 - n_{i,\downarrow})$$

Blocked levels

The Reduced BCS Hamiltonian:

$$\boxed{H_{BCS} = \sum_{i=1}^{N} \varepsilon_i b^{\dagger}_i b_i - G \sum_{i,j=1}^{N} b^{\dagger}_i b_j}$$



2. Richardson equations

The exact solution of the reduced BCS Hamiltonian was obtained by Richardson.

Ansatz: For a system with M pairs:

$$|M\rangle = \prod_{\nu=1}^{M} B_\nu^\dagger |vac\rangle \qquad B_\nu^\dagger = \sum_{i=1}^{N} \frac{b_i^\dagger}{\varepsilon_i - E_\nu}$$

provided that the pair energies E_ν follow the equations:

$$\boxed{\frac{1}{G} + \sum_{\mu(\neq\nu)=1}^{M} \frac{2}{E_\mu - E_\nu} - \sum_{i=1}^{N} \frac{1}{\varepsilon_i - E_\nu} = 0} \qquad (\nu = 1,\ldots,M)$$

The total energy of the system is given by $E = \sum_{\nu=1}^{M} E_\nu$

2-D electrostatic analogy:

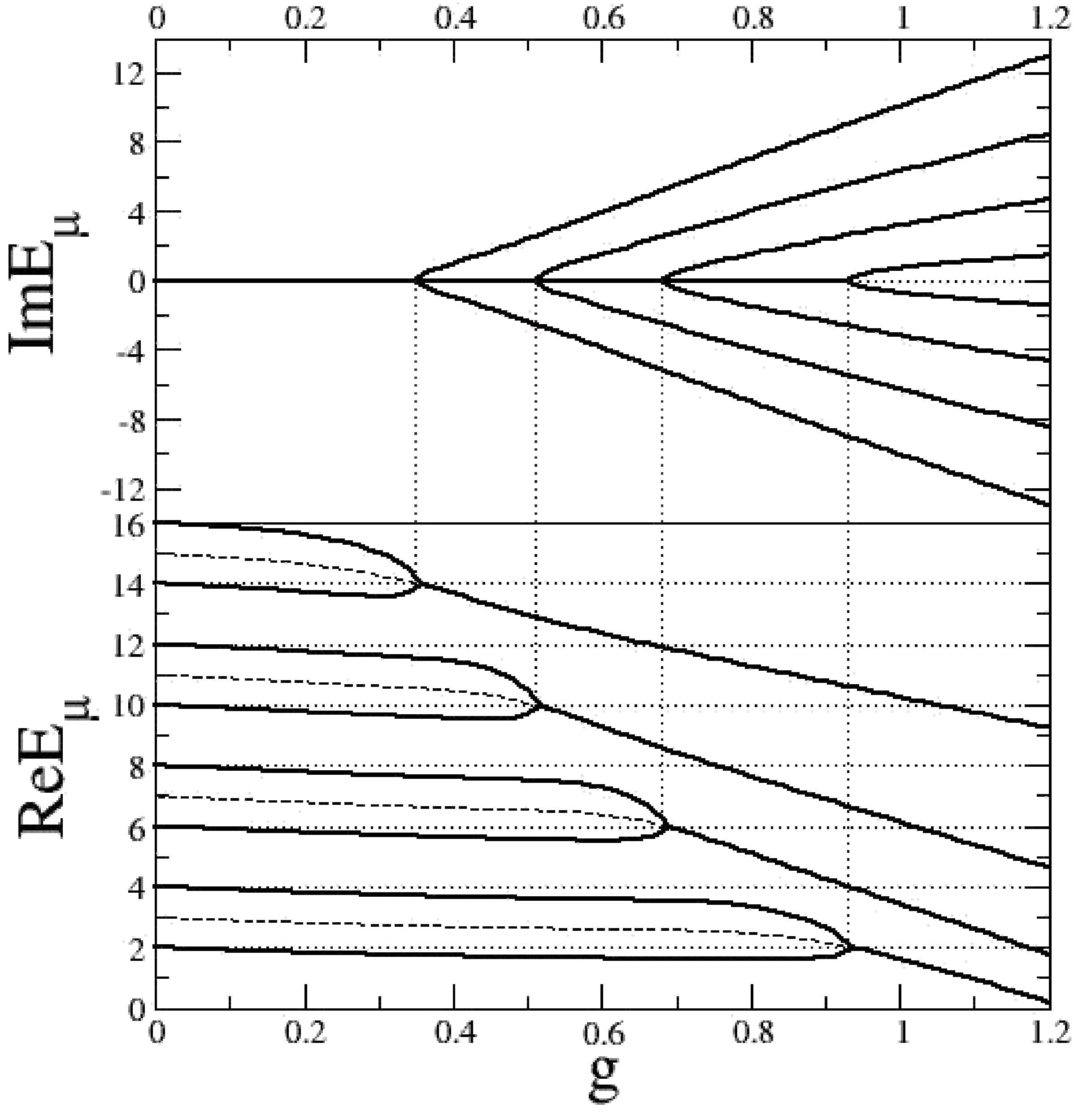
$$F[E_\nu] \equiv -\frac{1}{2G} + \sum_{\mu(\neq\nu)=1}^{M} \frac{1}{E_\nu - E_\mu} - \sum_{i=1}^{N} \frac{1/2}{E_\nu - \varepsilon_i} = 0$$

Uniform electric field parallel to the real axis

Mutual repulsion of charges +1

Attraction of N fixed charges –1/2

Evolution of the real and imaginary parts of $E_\mu(g)$ in units of $d = \omega/N$ for $N = 16$.



The existence of complex solutions of the Richardson equations is an indication of the superconducting properties of the Ground State.

3. Integrability of the BCS Hamiltonian

We can transform the BCS Hamiltonian into a spin Hamiltonian as follows:

$$b_i^\dagger = \sigma_i^-$$

$$b_i = \sigma_i^+$$

$$b_i^\dagger = \frac{1}{2}\left(1-\sigma_i^z\right)$$

$$H_{BCS} = H_{XY} + \frac{1}{2}\sum_{i=1}^{N}\varepsilon_i + G\left(\frac{N}{2} - M\right)$$

$$H_{XY} = -\sum_{i=1}^{N}\varepsilon_i t_i^z - \frac{G}{2}\left(T^+T^- + T^-T^+\right)$$

where $t_i^\pm = \sigma_i^\pm$, $t_i^z = \dfrac{\sigma_i^z}{2}$

$$T^a = \sum_{i=1}^{N} t_i^a \qquad (a = +,-,z)$$

Rivas, Cambiaggio and Sarraceno constructed the conserved quantities operators

$$\boxed{R_i = -t_i^z - 2G\sum_{j(\neq i)=1}^{N}\frac{\mathbf{t}_i\cdot\mathbf{t}_j}{\varepsilon_i - \varepsilon_j} \qquad (i = 1,\dots,N)}$$

$$\left[H_{BCS,}R_i\right] = \left[R_{i,}R_j\right] = 0$$

The eigenvalues of these operators, using the Richardson equations, are:

$$R_i\left|M\right\rangle = \lambda_i\left|M\right\rangle$$

$$\lambda_i = -\frac{1}{2} + G\left(\sum_{\nu=1}^{M}\frac{1}{\varepsilon_i - E_\nu} - \frac{1}{2}\sum_{j(\neq i)=1}^{N}\frac{1}{\varepsilon_i - \varepsilon_j}\right)$$

4. Continuum limit: BCS equations

In the $N \to \infty$ limit we assume that $g = G/N,\ M/N$ are fixed.

Level energies: $\varepsilon_i \to \varepsilon \quad \in \quad \Omega = (-\omega, \omega) \quad - \rho(\varepsilon)$

Pair energies: $E_\nu \to \xi \quad \in \quad \Gamma \quad r(\xi)$

$M = \int_\Gamma r(\xi) |d\xi|$ ⟶ Number of pairs in the arcs

$E = \int_\Gamma \xi r(\xi) |d\xi|$ ⟶ Total energy of the system

Richardson equations' continuum limit:

$$\int_\Omega \frac{\rho(\varepsilon) d\varepsilon}{\varepsilon - \xi} - P \int_\Gamma \frac{r(\xi') |d\xi'|}{\xi' - \xi} - \frac{1}{2G} = 0 \qquad \xi \in \Gamma$$

We introduce an electric analytic field $h(\xi)$ outside Γ and the interval Ω such that:

$$r(\xi) |d\xi| = \frac{1}{2\pi i} \left(h_+(\xi) - h_-(\xi) \right) d\xi \qquad \xi \in \Gamma$$

The electrostatic field presents a discontinuity proportional to the superficial density of charge when crossing a surface.

We consider the following expression for the field $h(\xi)$:

$$h(\xi) = R(\xi) \int_\Omega \frac{\varphi(\varepsilon) d\varepsilon}{\varepsilon - \xi} \qquad R(\xi) = \left[\prod_{k=1}^{K} (\xi - a_k)(\xi - b_k) \right]^{1/2}$$

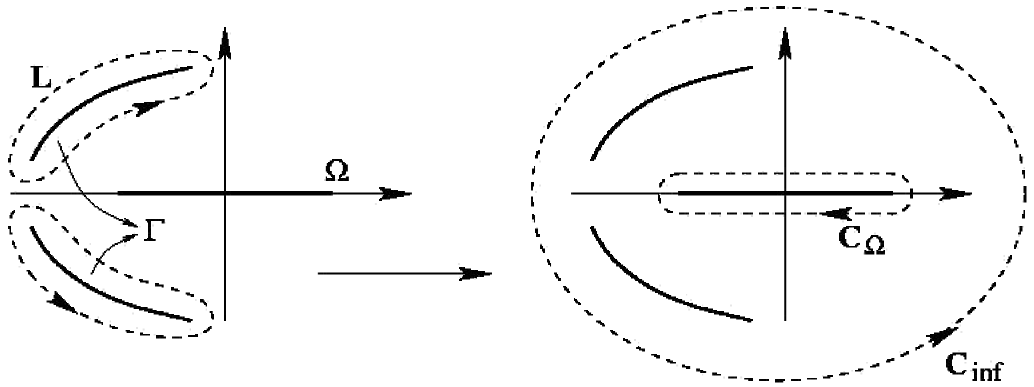
Number of arcs

Extremes of the arcs

Imposing that $h(\xi)$ is constant at infinity

$$\boxed{\int_\Omega \varepsilon^\ell \varphi(\varepsilon) = 0 \qquad 0 \le \ell < K - 1}$$

and deforming the contours of integration:



$$P \int_\Gamma \frac{r(\xi')|d\xi'|}{\xi - \xi'} = \frac{1}{2\pi i} \int_L \frac{h(\xi')d\xi'}{\xi - \xi'} = \frac{1}{2\pi i} \int_L \frac{d\xi' R(\xi')}{\xi - \xi'} \int_\Omega \frac{\varphi(\varepsilon)d\varepsilon}{\varepsilon - \xi'} =$$

$$= -\int_\Omega \frac{\varphi(\varepsilon)R(\varepsilon)d\varepsilon}{\varepsilon - \xi} + \int_\Omega \varepsilon^{K-1} \varphi(\varepsilon)d\varepsilon \quad \xi \in \Gamma$$

The solution of the continuum Richardson equations was derived by Gaudin:

$$\varphi(\varepsilon) = \frac{\rho(\varepsilon)}{R(\varepsilon)} \Rightarrow \begin{cases} \int_\Omega \varepsilon^\ell \frac{\rho(\varepsilon)}{R(\varepsilon)} = 0 \qquad 0 \le \ell < K-1 \\ \int_\Omega \varepsilon^{K-1} \frac{\rho(\varepsilon)}{R(\varepsilon)} = \frac{1}{2G} \end{cases}$$

Ground State BCS equations:

For the Ground state we assume a single arc, with the extremes of the arcs at the points:

$$\mathrm{K} = 1 \longrightarrow \begin{cases} a \equiv \varepsilon_0 - i\Delta \\ b \equiv \varepsilon_0 + i\Delta \end{cases}$$

$$\frac{1}{2G} = \int_\Omega \frac{\rho(\varepsilon)d\varepsilon}{\sqrt{(\varepsilon-\varepsilon_0)^2 + \Delta^2}}$$

GAP EQUATION

$$M = \int_\Omega \left(1 - \frac{\varepsilon - \varepsilon_0}{\sqrt{(\varepsilon-\varepsilon_0)^2 + \Delta^2}} \right) \rho(\varepsilon)d\varepsilon$$

$$E = -\frac{\Delta^2}{4G} + \int_\Omega \left(1 - \frac{\varepsilon - \varepsilon_0}{\sqrt{(\varepsilon-\varepsilon_0)^2 + \Delta^2}} \right) \rho(\varepsilon)\varepsilon d\varepsilon$$

$$\Delta = 2\Delta_{BCS} \qquad \varepsilon_0 = 2\mu \qquad \rho(\varepsilon) = \frac{1}{4} n\left(\frac{\varepsilon}{2}\right)$$

5. Numerical results

5.1. Two-level model

$$\rho(\varepsilon) = \frac{N}{4}[\delta(\varepsilon+\varepsilon_1)+\delta(\varepsilon-\varepsilon_1)] \qquad g \equiv GN$$

Superconducting phase $g \geq \varepsilon_1$:

GAP EQUATION $\longrightarrow$ $\varepsilon_1^2 + \Delta^2 = g^2$

NUMBER EQUATION $\longrightarrow$ $\varepsilon_0 = 0$

ENERGY EQUATION $\longrightarrow$ $E = -\frac{N}{4g}\left(\varepsilon_1^2 + g^2\right)$

Normal phase $g \leq \varepsilon_1$: $\Delta = 0 \;\Rightarrow$ Closed curves $\varepsilon_0 \neq 0$

$$r(\xi)\left|d\xi\right| = s(\xi)d\xi$$

$$s(\xi) = \frac{i}{\pi}\left[\frac{1}{2G} + \int_{\omega}\frac{\rho(\varepsilon)d\varepsilon}{\varepsilon-\xi} - \int_{C\omega}\frac{\rho(\varepsilon)d\varepsilon}{\varepsilon-\xi}\right] \qquad \xi \in \Gamma$$

Imposing zero density at the extreme of the closed curve:

$$s(\varepsilon_0) = 0 \quad \Longrightarrow \quad \varepsilon_0 = -\varepsilon_1\sqrt{1-\frac{g}{\varepsilon_1}}$$

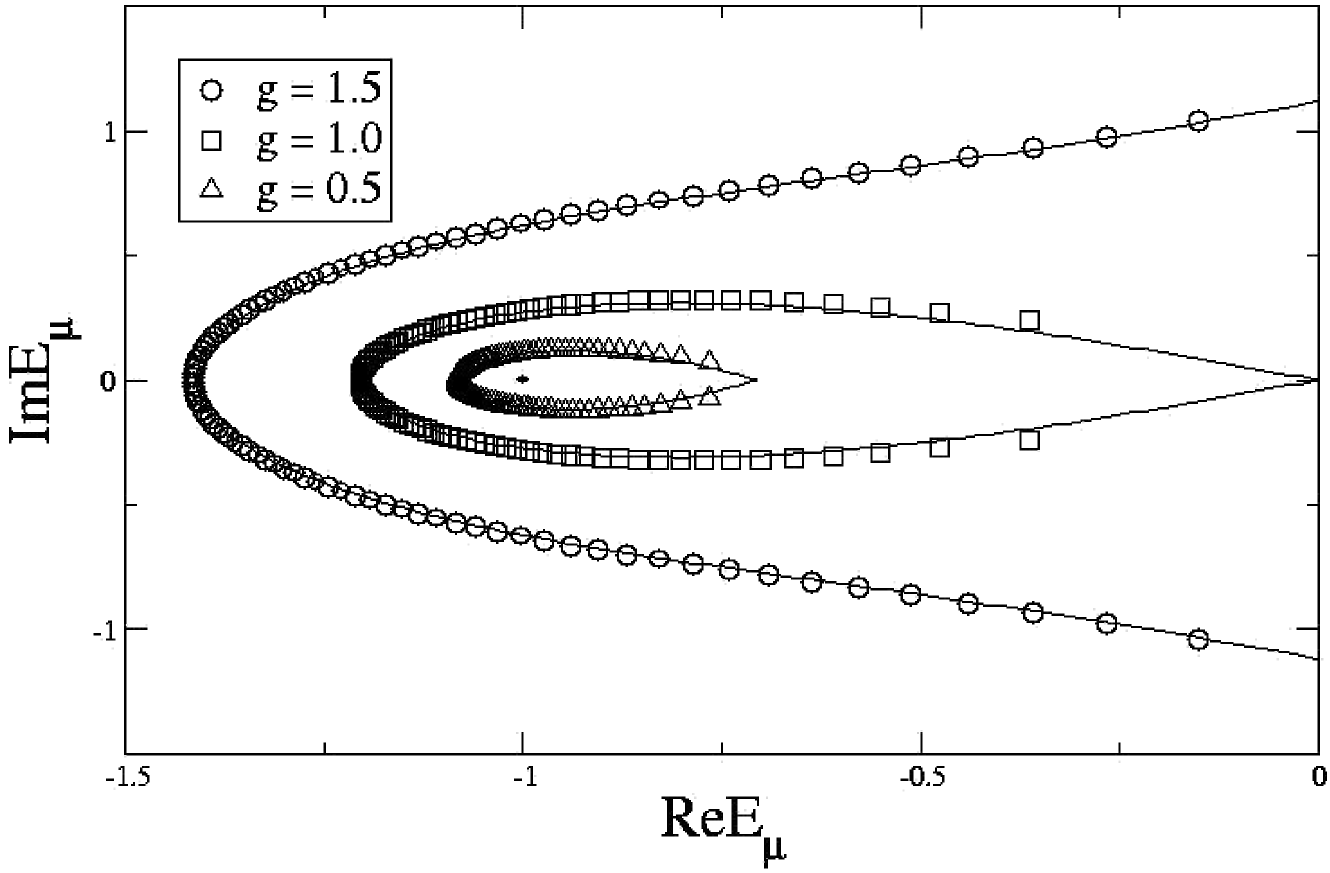
NUMBER EQUATION

$$M = \int_{\Gamma} d\xi s(\xi) = \int_{\omega} d\varepsilon 2\rho(\varepsilon) = \frac{N}{2}$$

ENERGY EQUATION

$$E = \int_{\Gamma} d\xi\xi s(\xi) = \int_{\omega} d\varepsilon 2\varepsilon\rho(\varepsilon) = -\frac{N}{2}\varepsilon_1$$

Plot of the solutions of Richardson equations for the two-level model for different values of the coupling g. The lines represent the analytic results, and the numerical results are for a system with $M = 100$ pairs.



$g = 1$ represents a phase transition between a normal phase and a superconducting phase.

The extremes of the arcs approach their continuum limit $\varepsilon_0 + i\Delta$ through a power law function:

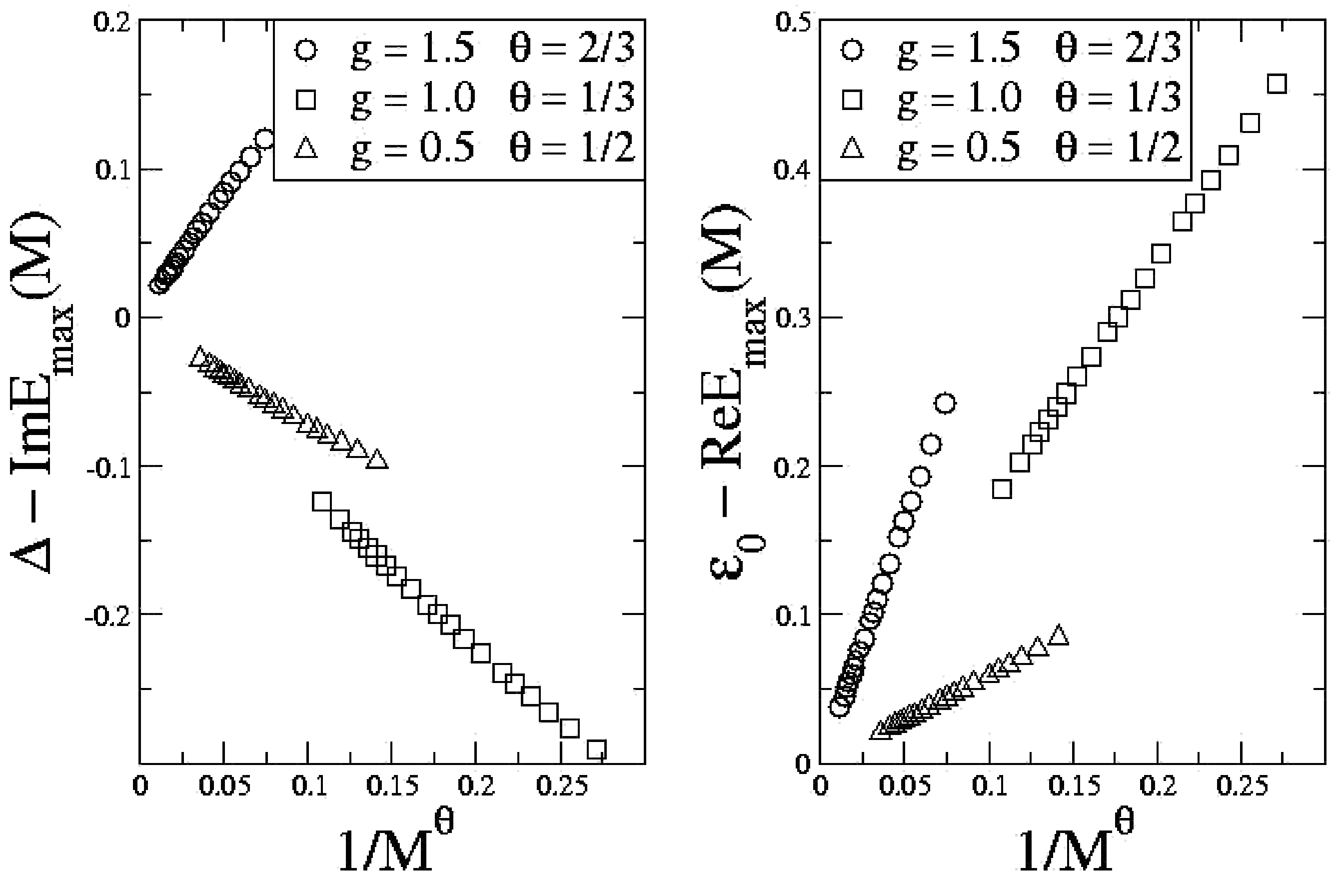
$$E_{\max}(M) - (\varepsilon_0 + i\Delta) \sim M^{-\theta} \qquad \theta = \begin{cases} 2/3 & g > \varepsilon_1 \\ 1/3 & g = \varepsilon_1 \\ 1/2 & g < \varepsilon_1 \end{cases}$$

The density of roots at the extreme of the arcs:

$$r(E_{\max}) \sim AM(\delta\xi)^{\nu} \qquad \nu = \begin{cases} 1/2 & g > \varepsilon_1 \\ 2 & g = \varepsilon_1 \\ 1 & g < \varepsilon_1 \end{cases}$$

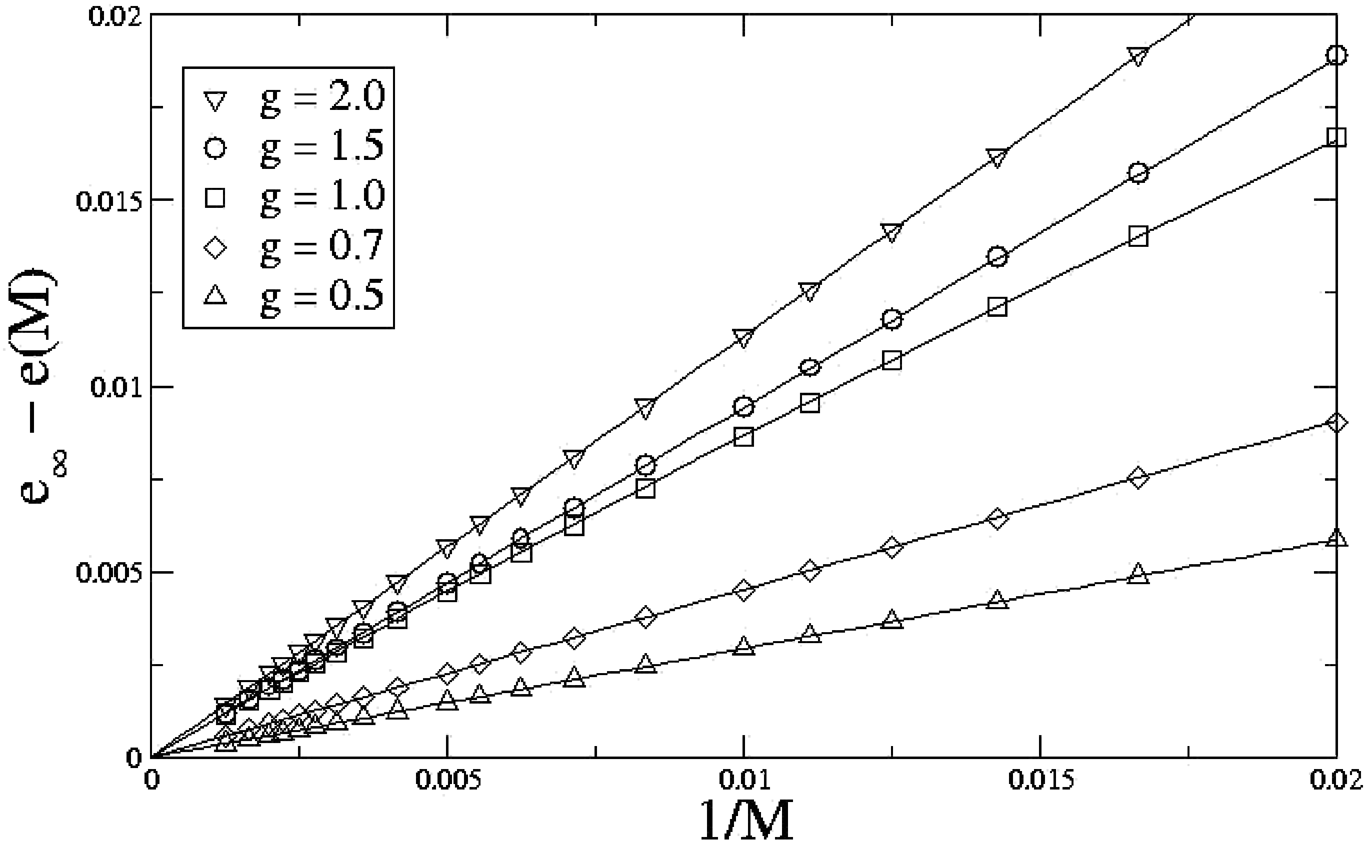
Assuming one root in the interval $|\delta\xi|$:

$$1 = r(E_{\max})|\delta\xi| \sim AM|\delta\xi|^{\nu+1} \quad \rightarrow \quad \delta\xi \sim M^{-\frac{1}{\nu+1}} \quad \theta = \frac{1}{\nu+1}$$



The energy per pair $e(M) = E(M)/M$ approaches its thermodynamic limit following the relations:

$$e_\infty - e(M) = \begin{cases} \left(g - \frac{1}{2}\Delta\right)\frac{1}{M} & g > \varepsilon_1 \\ \varepsilon_1\left(\frac{1}{M} - \frac{A}{M^{4/3}}\right) & g = \varepsilon_1 \qquad A = 0.62258 \\ \left(\varepsilon_1 - |\varepsilon_0|\right)\frac{1}{M} & g < \varepsilon_1 \end{cases}$$



5.2. Equally spaced model

$$\rho(\varepsilon) = \rho_0 = \frac{N}{4\omega} \quad \varepsilon \in (-\omega, \omega) \qquad d = \frac{\omega}{N} = \frac{2\omega_D}{N} \qquad g \equiv \frac{GN}{\omega}$$

Debye frequency cut-off

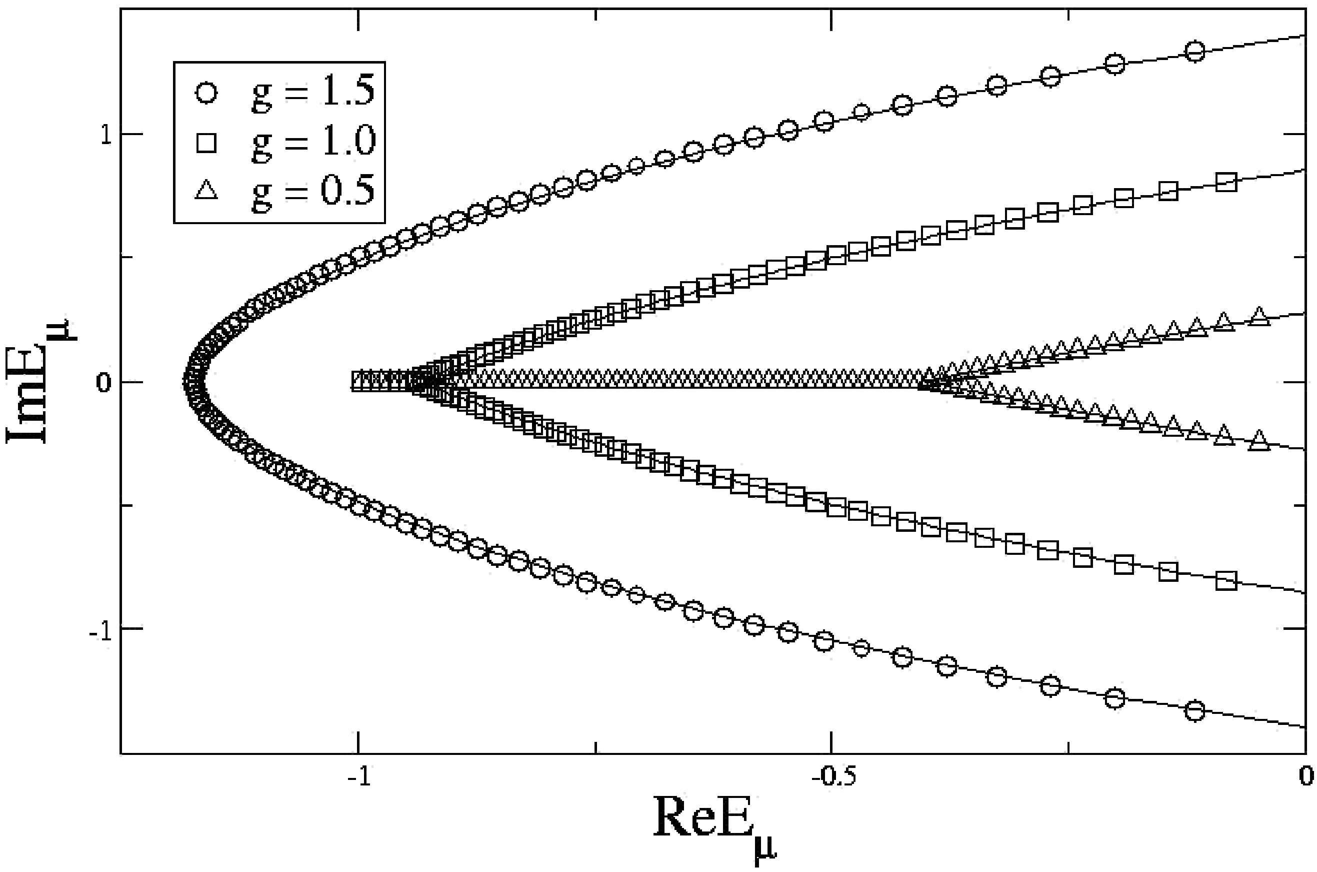
We are always in a superconducting phase

GAP EQUATION $\qquad \Delta = \dfrac{\omega}{\sinh(1/g)}$

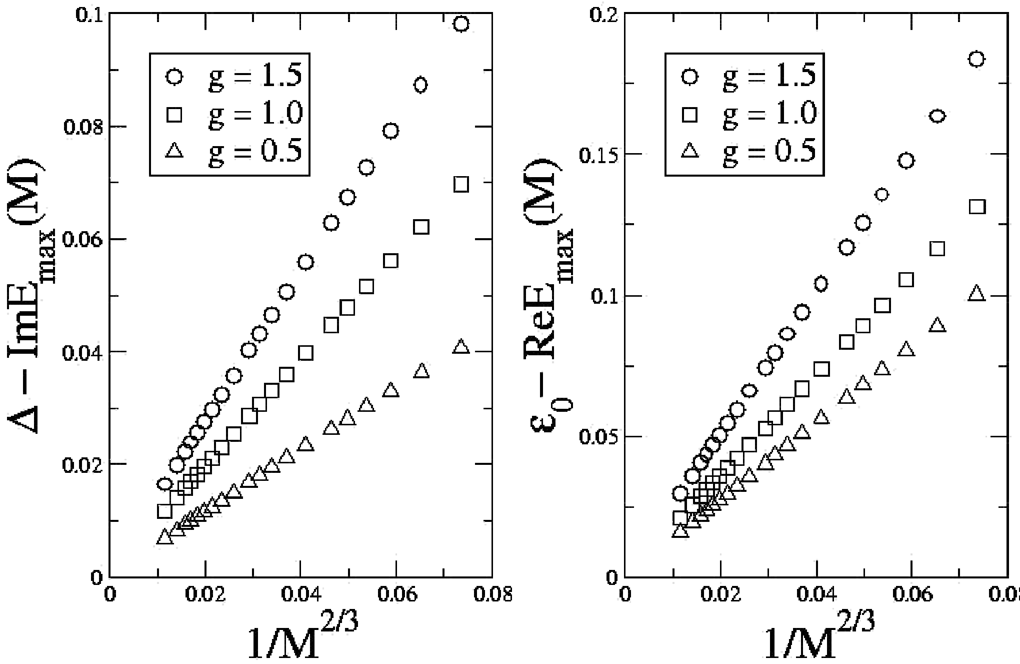
NUMBER EQUATION $\qquad \varepsilon_0 = 0$

ENERGY EQUATION

$$E_C = -\frac{\omega^2}{4d}\left[\sqrt{1+\left(\frac{\Delta}{\omega}\right)^2} - 1\right] + \frac{GN}{2} \quad \sim \quad -\frac{\Delta_{BCS}^2}{2d}$$

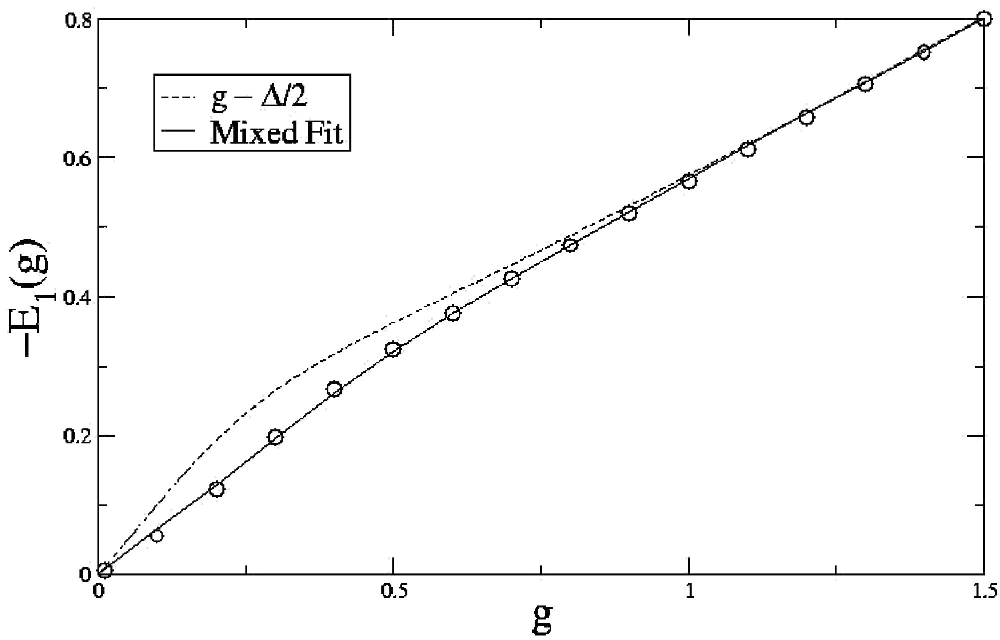


The extremes of the arcs approach their thermodynamic limit with a power law function with $\theta = 2/3$



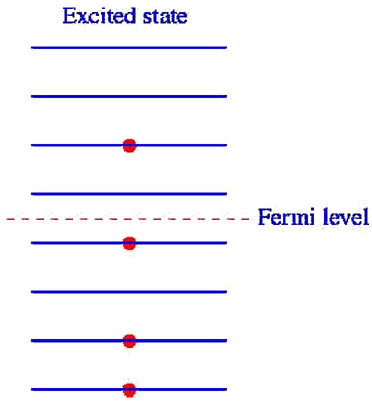
The condensation energy goes to the large-N limit as $1/M$, and the slope variation as function of g is:

$$-E_1(g) = \left(g - \frac{\Delta}{2\omega}\right)\frac{M_{complex}}{M} + (A + Bg)\frac{M_{real}}{M} \qquad \begin{cases} A = 0.6735 \\ B = -0.1729 \end{cases}$$



6. Excitations: Pics

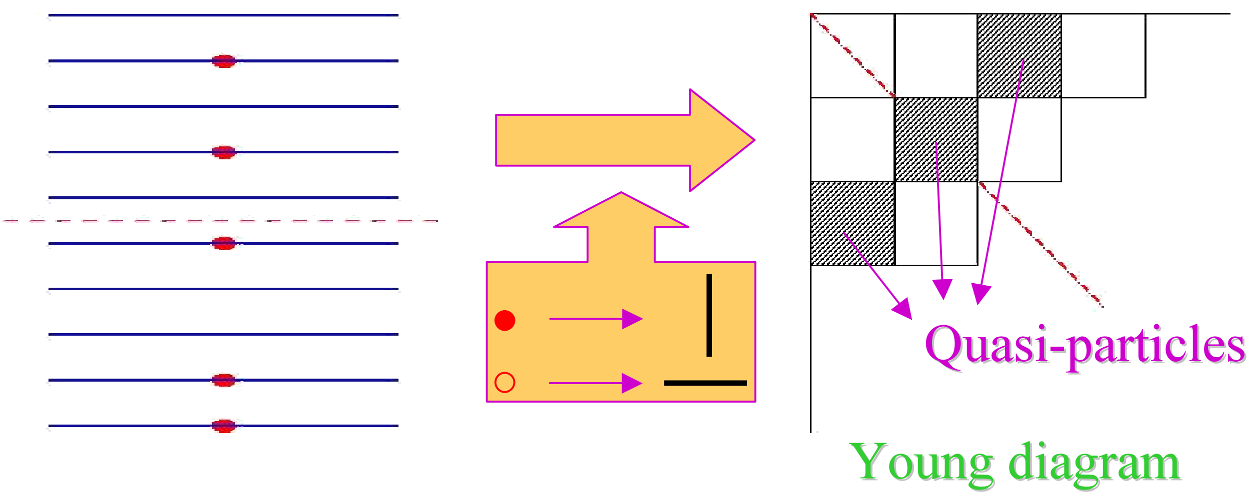
Excited states correspond to particle-hole excitations of pairs from the Fermi Sea at $g = 0$.



1. Quasi-particles of the system are not described by simple particle-hole excitations.
2. Quasi-particles are associated to those pair energies remaining finite in the limit $g \to \infty$.
3. Given the particle-hole representation of the excited state we can know the number of quasi-particles.

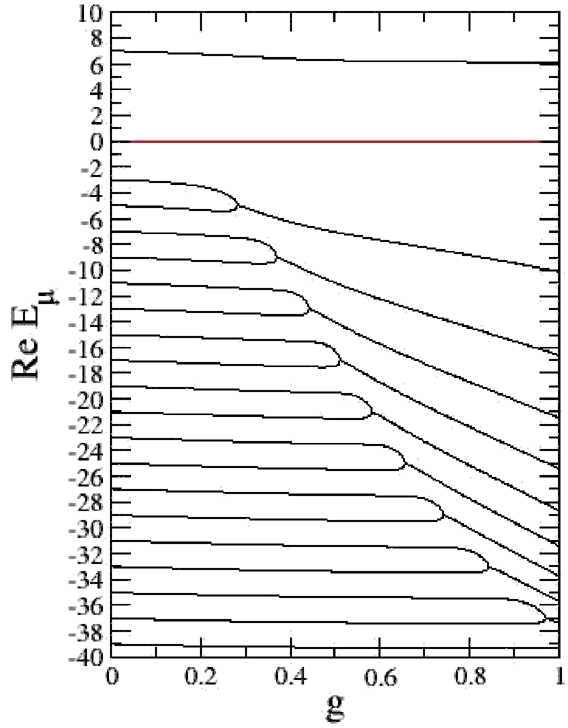
The excited states will show all the features we did not find in the Ground State properties:

1. Several arcs in the large-N limit
2. Crossing of pair energies

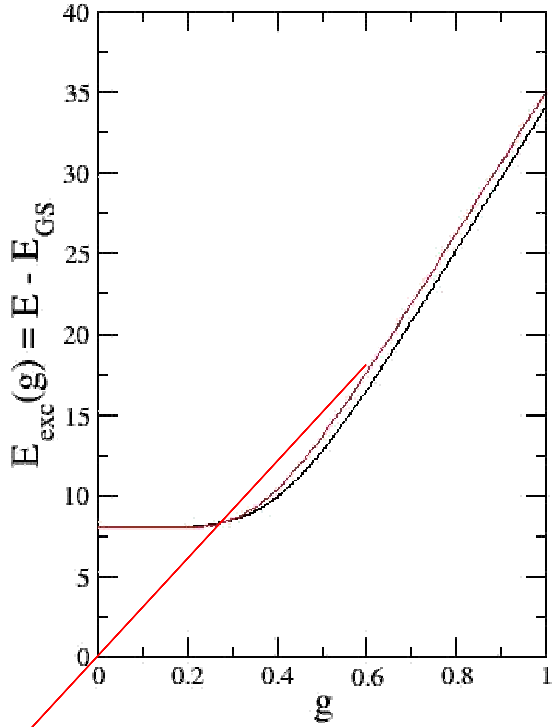


A particle-like excitation:

(1;7)



1 particle



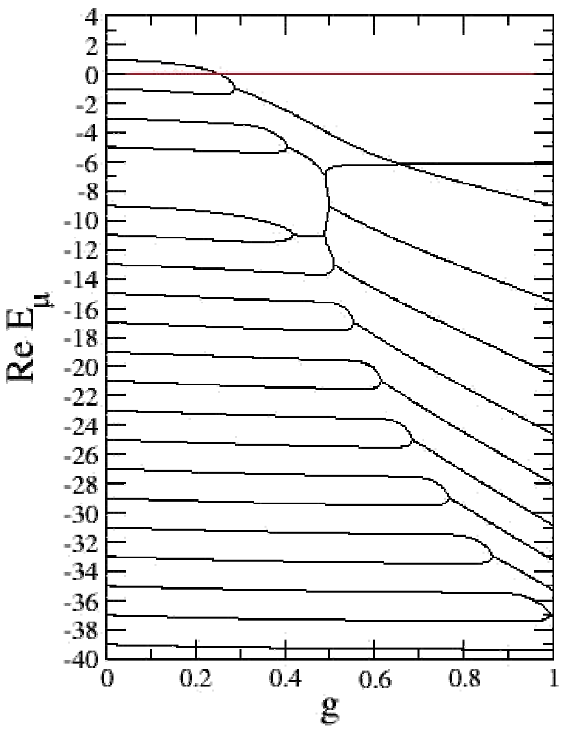
A hole-like excitation:

$$E_{exc}(g) = \sqrt{\varepsilon_0^2 + \Delta^2}$$

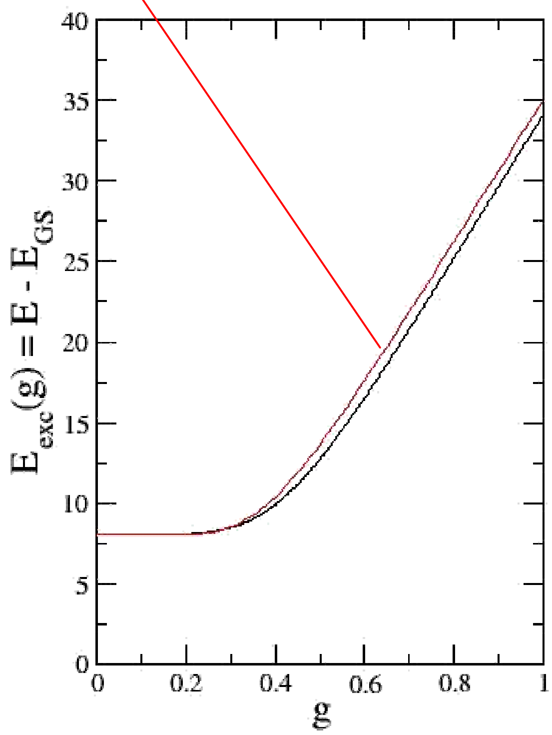
$\varepsilon_0 = 8$

$$\Delta_{bulk} = \frac{Nd}{\sinh(1/g)}$$

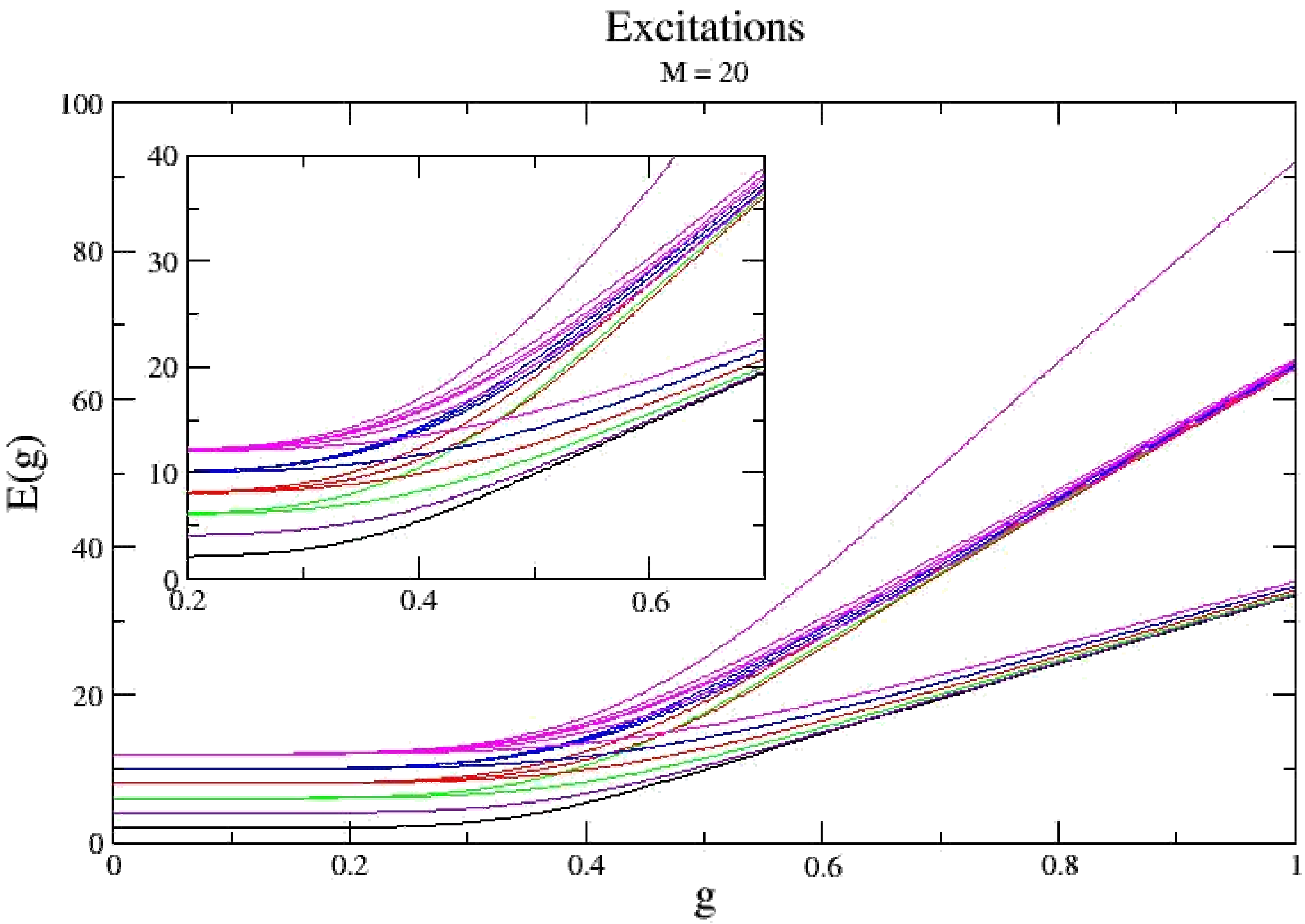
(7;1)



1 hole

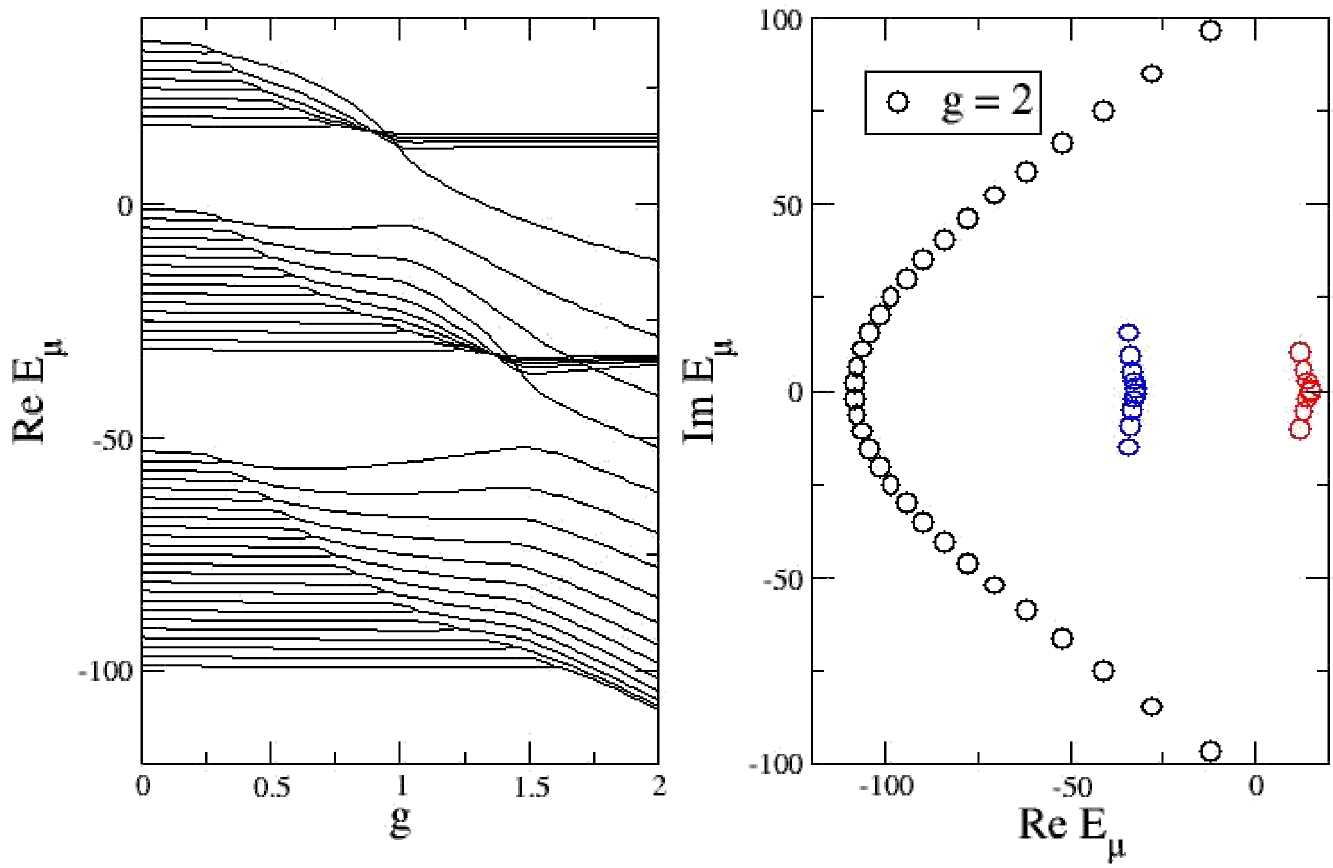


1. The excitations rearrange themselves to merge into states of defined energy equal to integers of the gap, in the large g limit.
2. The integer corresponds to the number of quasi-particles.



Several arcs in the large-N limit:

The pairs distributed arbitrarily in packages may give rise to several arcs, as shown in the figure:



System with $M = 50$ pairs distributed in the following configurations of

holes-particles-holes-particles-...

0 24 – 10 16 – 8 10 – 32 0

7. Conclusions and prospects

1. We have presented the exact solution to the reduced BCS Hamiltonian given by Richardson equations.

2. The Richardson equations were solved in the thermodynamic limit. In particular, the Ground State of the system was thoroughly studied.

3. The solutions of Richardson equations arrange into arcs. The imaginary part of the extreme points is twice the BCS gap. The real part is twice the chemical potential.

4. The scaling behavior of the ground state energy and the gap were presented by comparing analytical and numerical results for the two-level and equally spaced models.

PROSPECTS:

What does it play the role of the phase in the canonical ensemble formulation of superconductivity?

How are the excitations related to the Bogoliubov quasi-particles?

How do the excitations loose the high level of correlation they show?