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Generalised Heine-Stieltjes and Van Vleck polynomials associated with integrable BCS models

We will present new results concerning numerical methods to study integrable systems based on the Bethe Ansatz/Ordinary Differential Equation (BA/ODE) correspondence. We will discuss how this approach can be applied to four cases of exactly solvable Bardeen-Cooper-Schrieffer (BCS) pairing models in their degenerate two-level limit. These are the s-wave pairing model, the p+ip-wave pairing model, the p+ip pairing model coupled to a bosonic molecular pair degree of freedom, and a d + id-wave pairing model with additional interactions. The zeros of the generalised Heine-Stieltjes polynomials provide solutions of the corresponding Bethe ansatz equations. We compare the roots of the ground states with curves obtained in the continuum limit.

Outline

- Zeros of polynomials, BA/ODE correspondence,
- Integrable BCS models
- Generalised Heine-Stieltjes and Van Vleck polynomials, Numerical methods
- Numerical calculation of the roots for the four degenerate two-level models, comparison with continuum limit
- Concluding remarks

BA/ODE correspondence

- The correspondence between electrostatic models and zeros of polynomials has a very long history :
  Heine (1878), Stieltjes (1885), Bôcher (1897), Van Vleck (1898), Polya (1912), Szégo (1959), Case (1980)
- Many polynomials were studied such Laguerre, Jacobi, ...
- Generalized Lamé equation, their polynomial and zeros were studied :
  Zaheer and Alam (1976), Martinez-Finkelshtein (2002), Bourget (2010),Borcea (2007), Shapiro (2010,2011)
- Higher order differential operators : Bergkvist (2007)
- Polynomial solutions using Bethe Ansatz approach : Zhang (2012), Zhang and Agboola (2012)

The zeros $\{y_j\}$ of the Hermite polynomials $H_n(y)$ satisfy the Bethe Ansatz

$$y_j = \sum_{1\leq k\leq n, k\neq j} \frac{1}{y_j - y_k}$$

The generalized Lamé equation

$$A_2(z)Q''(z) + A_1 Q'(z) + A_0(z)Q(z) = 0$$

- A_2 and A_0 are real polynomials of degree L and $L-1$
- (L=3 Heun) and ($A_1 = \frac{1}{2}A_2'$ Lamé)
- A_0 and Q are the Van Vleck and Stieltjes polynomials

- The BA/ODE correspondence was discussed by many authors :
  -Gaudin (1968) : Relation between s-wave model and the confluent Heun equation
  -Enol'skii, Kuznetsov and Salerno (1993), Ulyanov and Zaslavskii (1992)

- However, the idea of using this correspondence to provide numerical methods to study such systems is much more recent. The roots are now given in terms of the zeros of polynomials that satisfy a ODE

- Faribault, Araby, Strater and Gritsev (2011,2012) : Riccati equation (first order), track the roots of the ground state from $g = 0$, barycentric
- Pan F, Bao L, Zhai L, Cui X and Draayer J P (2011) : Linear second order differential equation, all the roots, monomial

BCS models : Richardson-Gaudin (s-wave)

$$H_s = \sum_{j=1}^{L} \varepsilon_j N_j - G \sum_{j,k}^{L} b_j^\dagger b_k$$

- The parameters ε_i is the single particle energy levels, L the number of levels and M the total number of Cooper pairs.
- The hard-core boson operators $b_j^\dagger$, b_k and $N_j = b_j^\dagger b_j$ satisfy

$$(b_j^\dagger)^2 = 0, \quad [b_j, b_k^\dagger] = \delta_{jk}(1 - 2N_j), \quad [b_j, b_k] = [b_j^\dagger, b_k^\dagger] = 0$$

- Bardeeen, Cooper and Schrieffer (1957) : BCS model
- Richardson and Sherman (1963,1964) : Exact Bethe Ansatz
- Gaudin (1968) : Continuum limit, electrostatic analogy, BA/ODE

$$\tau_j = -\frac{1}{2G}(N_j - I) + \sum_{k \neq j}^{L} \frac{\theta_{jk}}{k_i - k_k},$$

$$\theta = b^\dagger \otimes b + b \otimes b^\dagger + \frac{1}{2}(N_j - I) \otimes (N_j - I)$$

- Cambiaggio, Rivas and Saraceno (1997) : Integrability
- Links, Zhou, McKenzie and Gould (2003) : Quantum inverse scattering method and Algebraic Bethe Ansatz

$$\sum_{i=1}^{L} \frac{1}{y_l - \varepsilon_i} - 2\sum_{j \neq l}^{M} \frac{1}{y_l - y_j} + \frac{1}{G} = 0, E = \sum_{j=1}^{M} y_j$$

- Conformal field theory, Quench, Correlation functions
- Numerical : Roman, Sierra and Dukelsky (2002), Domínguez, Esebbag and Dukelsky (2006)

p+ip-wave model and p+ip with bosonic degree of freedom

$$H_p = \sum_{i=1}^{L} \varepsilon_i N_i - G \sum_{j<k}^{L} \sqrt{\varepsilon_j \varepsilon_k}(b_j^\dagger b_k + b_k^\dagger b_j).$$

- Dunning, Ibañez, Links , Sierra and Zhao (2010), Rombouts, Dukelsky and Ortiz (2010) : Integrability, continuum, mean field, numerical, correlation functions, phase diagram

$$H_{pb} = H_p - F^2 G N_0 - FG \sum_{j=1}^{L} \sqrt{\varepsilon_i}(b_0 b_j^\dagger + b_0^\dagger b_j)$$

- b_0, $b_0^\dagger$ satisfy $[b_0, b_0^\dagger] = I$ and $N_0 = b_0^\dagger b_0$
- Dunning, Isaac, Links and Zhao (2011)

Extended d+id-wave model

$$H_d = \sum_{i=1}^{L} \varepsilon_i N_i - G \sum_{j,k=1}^{L} \varepsilon_j \varepsilon_k (b_j^\dagger b_k + b_j b_k^\dagger + 2N_j N_k)$$

- Ian Marquette and Jon Links, Nucl. Phys. B 866 378-390 (2013)
- Related by a duality relation with the s-wave model,
- energy spectrum given by double sum of the roots
- Continuum limit of Bethe Ansatz equations, mean field

Bethe Ansatz equations

$$\sum_{i=1}^{L} \frac{\rho_i}{y_l - \varepsilon_i} - 2\sum_{j\neq l}^{M} \frac{1}{y_l - y_j} + \frac{A}{y_l^2} + \frac{B}{y_l} + C = 0, \qquad l = 1, ..., M.$$

- $C = G^{-1}$ and $A = B = 0$
- $B = G^{-1} - L + 2M - 1$ and $A = C = 0$
- $C = 0,\ B = G^{-1} + 2M - L - 1$ and $A = F^2$
- $C = 0,\ B = 2M - 2 - L$ and $A = (2G)^{-1} - \sum_{i=1}^{L} \varepsilon_i$

Generalized Heine-Stieltjes and Van Vleck polynomials

- Ian Marquette and Jon Links, J.Stat. Mech. P08019 (2012)
- Approach we follow : Second order differential equation, monomial and all the roots
- The systems studied previously using the polynomial approach belong to the class of coupled nonlinear algebraic (Bethe Ansatz) equations of the form

$$\sum_{i=1}^{L} \frac{\rho_i}{y_l - \varepsilon_i} - 2\sum_{j \neq l}^{M} \frac{1}{y_l - y_j} + C + Dy_l = 0, \qquad l = 1, ..., M$$

  where C, D, ρ_i and ε_i are real parameters
- Bethe Ansatz equations of p+ip and d+id models belong to a different class

- We start by constructing the following polynomials

$$Q(z)=\prod_{j=1}^{M}(z-y_j), \quad P(z)=\prod_{i=1}^{L}(z-\varepsilon_i).$$

- They satisfy the following relations

$$\frac{Q''(y_l)}{Q'(y_l)}=2\sum_{j\neq l}^{M}\frac{1}{y_l-y_j}, \quad \frac{P'(y_l)}{P(y_l)}=\sum_{i=1}^{L}\frac{1}{y_l-\varepsilon_i}.$$

- We introduce a polynomial $W(z)$ which is of order $L-1$ such that for the set of real parameters ρ_i and ε_i it satisfies

$$\frac{W(z)}{P(z)}=\sum_{i=1}^{L}\frac{\rho_i}{z-\varepsilon_i},$$

- These relations can be used to construct

$$\frac{A}{y_l^2}+\frac{B}{y_l}+C+\frac{W(y_l)}{P(y_l)}-\frac{Q''(y_l)}{Q'(y_l)}=0.$$

- The polynomial $Q(z)$ vanishes at the solutions y_l of the Bethe Ansatz equations
- The order $|A_j|$ of the polynomial $A_j(z)$ depends on when the parameters A, B, C vanish

$$A_2(z)Q''(z) + A_1(z)Q'(z) = A_0(z)Q(z),$$

TABLE: Cases

A	B	C	A_2	A_1	$\|A_2\|$	$\|A_1\|$	$\|A_0\|$
$\neq 0$	$\neq 0$	$\neq 0$	z^2P	$-(A + Bz + Cz^2)P$ $-z^2W$	$L+2$	$L+2$	$L+1$
$\neq 0$	$\neq 0$	$= 0$	z^2P	$-(A + Bz)P - z^2W$	$L+2$	$L+1$	L
$\neq 0$	$= 0$	$\neq 0$	z^2P	$-(A + Cz^2)P - z^2W$	$L+2$	$L+2$	$L+1$
$\neq 0$	$= 0$	$= 0$	z^2P	$-AP - z^2W$	$L+2$	$L+1$	L
$= 0$	$\neq 0$	$\neq 0$	zP	$-(B + Cz)P - zW$	$L+1$	$L+1$	L
$= 0$	$\neq 0$	$= 0$	zP	$-BP - zW$	$L+1$	L	$L-1$
$= 0$	$= 0$	$\neq 0$	P	$-CP - W$	L	L	$L-1$

- We start by taking the following expansions (where M and L are fixed) of the generalized Heine-Stieljes and Van Vleck polynomials ($\alpha_M = 1$)

$$Q(z) = \sum_{j=0}^{M} \alpha_j z^j, \quad A_0(z) = \sum_{j=0}^{|A_0|} \beta_j z^j$$

- α_j and β_j are to be determined numerically by inserting the expansion
- We have adapted a code using Mathematica to implement the calculations
- The solutions correspond to coefficients for the ground states and the excited states
- We can observe that the order of these coefficients can differ greatly

- We can thus for each generalized Heine-Steiljes compute the zeros
- The ground states can be identified using the formula for the energy (in the case of s-model or p+ip with α_{M-1})
- For our numerical investigations we will study degenerate two-level models, where each of the distinct levels ε_1 and ε_2 have have degeneracy $L/2$

$$\frac{A}{y_l^2} + \frac{B}{y_l} + C - \frac{L}{2}\left(\frac{1}{\varepsilon_1 - y_l} + \frac{1}{\varepsilon_2 - y_l}\right) - 2\sum_{j\neq l}^{M} \frac{1}{y_l - y_j} = 0$$

- Difficulty : numerical methods to find roots can have instabilities Wilkinson (1959), Farouki (1996) Corless and Watt (2004)
- This problem can even affect the structure of the roots (i.e. real vs. complex conjugate pairs)

2-level limit

- The degenerate two-level limit is obtained by setting

$$\varepsilon_j = \begin{cases} \varepsilon_1 & j \text{ odd}, \\ \varepsilon_2 & j \text{ even} \end{cases}$$

- The Hamiltonian may be expressed

$$H = L + 2\varepsilon_1 \mathcal{S}_1^z + 2\varepsilon_2 \mathcal{S}_2^2 - G(\mathcal{S}_1^+ + \mathcal{S}_2^+)(\mathcal{S}_1^- + \mathcal{S}_2^-)$$

$$\mathcal{S}_1^z = \frac{1}{2}\sum_{j \text{ odd}} (2N_j - I), \qquad \mathcal{S}_2^z = \frac{1}{2}\sum_{j \text{ even}} (2N_j - I),$$

$$\mathcal{S}_1^- = \sum_{j \text{ odd}} b_j, \qquad \mathcal{S}_2^- = \sum_{j \text{ even}} b_j,$$

$$\mathcal{S}_1^+ = \sum_{j \text{ odd}} b_j^\dagger, \qquad \mathcal{S}_2^+ = \sum_{j \text{ even}} b_j^\dagger$$

2-level limit

- Only provides a subset ($(L/2+1)^2$) of the spectrum for the Hilbert space of dimension 2^L
- They are the *unblocked symmetric states* i.e. invariant under the mutual interchange of the even (odd) subscripts (tensor products)
- Such model is useful in context of the numerical approach based on BA/ODE correspondence

$$\frac{1}{G} - \frac{L}{2}\left(\frac{1}{\varepsilon_1 - y_l} + \frac{1}{\varepsilon_2 - y_l}\right) - 2\sum_{j \neq l}^{M} \frac{1}{y_l - y_j} = 0$$

Continuum limit of BA equations

- If in the limit $L \to \infty$ the roots of the Bethe ansatz equations are densely distributed on a curve Γ in the complex plane, we obtain the singular integral equation

$$\frac{A}{y^2} + \frac{B}{y} + C + \int_\Omega d\varepsilon \frac{\rho(\varepsilon)}{y-\varepsilon} + P \int_\Gamma |dy'| \frac{2r(y')}{y'-y} = 0$$

where Ω denotes the interval of the real line where the energy levels ε lie, distributed according to a density $\rho(\varepsilon)$ such that $\int_\Omega d\varepsilon\, \rho(\varepsilon) = 1$

- It can be solved using complex analysis techniques
- The solution for Γ having end points $a = \epsilon - i\delta$ and $b = \epsilon + i\delta$

$$x = \mathcal{F}_1(a,b), \quad g = \mathcal{F}_2(a,b)$$

-We can obtained the equation of the arc (also closed curves)

- We set : $\gamma = \varepsilon_1 + \varepsilon_2$ and $\eta = \varepsilon_2\varepsilon_1$

$$(z^2 - \gamma z + \eta)Q'' + \left(\left(\frac{\gamma}{G} - L\right) z - \frac{1}{G}z^2 + \frac{1}{2}\gamma L - \frac{\eta}{G}\right) Q'$$
$$-(\beta_1 z + \beta_0)Q = 0$$

- From the first and second terms in the expansion of the polynomial $Q(z) = z^M - Ez^{M-1} + \ldots + (-1)^M \prod_{j=1}^M y_j$

$$\beta_1 = -\frac{M}{G}, \quad \beta_0 = -\left(\frac{\gamma}{G}M + \frac{E}{G} + M + LM - M^2\right).$$

- We take $\varepsilon_2 = 1$ and $\varepsilon_1 = -1$, $L = 100$, half-filling, $M = 50$, and introduce the scaled coupling constant $g = GL$.
- The results agree with the theoretical distribution curve in the large-L limit and previous numerical calculations
- The case $g = 1$ is identified as a critical point

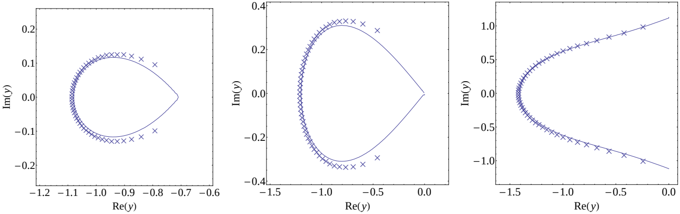

FIGURE: Roots for the ground state (a) $g = 1/2$, (b) $g = 1$, and (c) $g = 3/2$. Also shown are the theoretical curves for the large-L limit.

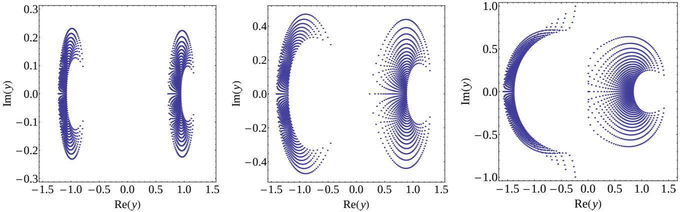

FIGURE: (a) $g = 1/2$, (b) $g = 1$, and (c) $g = 3/2$. In each case a total of 51 sets of roots are displayed, where each set contains 50 roots.

$$(z^3-\gamma z^2+\eta z)Q''+(\frac{\eta(-1+G(1+L-2M))}{G}+\frac{\gamma z(2-G(2+L-4M)}{2G}$$

$$+\frac{(-1+G-2GM)z^2}{G})Q'-(\beta_1 z+\beta_0)Q=0.$$

$$\beta_1=-\left(\frac{M}{G}+M^2\right),\quad \beta_0=-\left(\frac{E}{G}-\frac{\gamma M}{G}+\frac{\gamma LM}{2}-\gamma M^2\right).$$

- We consider the case $\varepsilon_2=1$, $\varepsilon_1=1/2$, $L=200$, and $M=50$.
- At MR line there is a change from an open curve to a closed curve, however all the roots collapse to the origin A
- Idenfied as a zeroth order quantum phase transition (as $g\to g_{MR}$ and $L\to\infty$ do not commute)
- At RG line the closed curve contract to a point at the origin

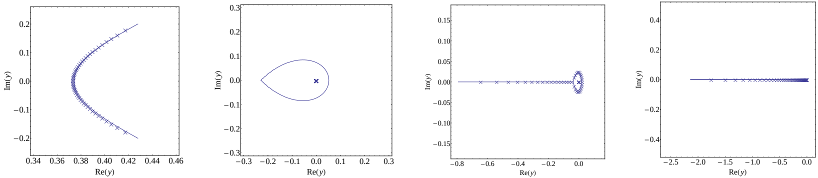

FIGURE: Roots for the ground state $g = 1/2$ (Weak coupling BCS), (b) $g = 4/3$ (Moore-Read line), (c) $g = 3/2$ (Weak pairing), and (d) $g = 2$ (Read-Green line).

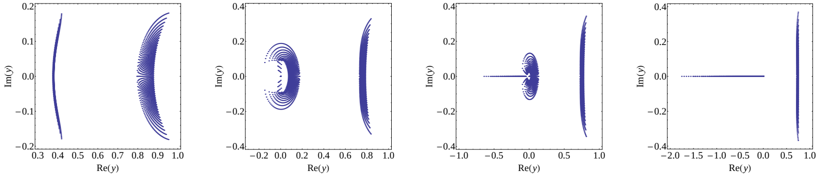

FIGURE: Roots for all unblocked symmetric states of the degenerate (a) $g = 1/2$, (b) $g = 4/3$, (c) $g = 3/2$, and (d) $g = 2$.

p+ip-wave model with bosonic degree of freedom

$$(z^4-\gamma z^3+\eta z^2)Q''+((F^2\gamma+\eta-\frac{\eta}{G}+\eta L-2\eta M)z-F^2\eta$$
$$+(\frac{\gamma}{G}-\frac{\gamma L}{2}+2\gamma M-F^2-\gamma)z^2+(1-\frac{1}{G}-2M)z^3)Q'$$
$$-(\beta_2 z^2+\beta_1 z+\beta_0)Q=0$$

$$\beta_2=M\left(\frac{-1}{G}-M\right),\beta_1=\left(\frac{2\gamma GM^2-2E-(-2(\gamma-F^2G)+\gamma GL)M}{2G}\right)$$

- The coefficient β_0 is more complicated than for the previous examples and involves a double sum
- $\varepsilon_2=1$ and $\varepsilon_1=1/2$, $L=32$, $M=L/2$ and $F=\sqrt{128}$
- Ground-state roots always lie on the negative real-axis and there are no qualitative changes as the coupling parameter g is varied

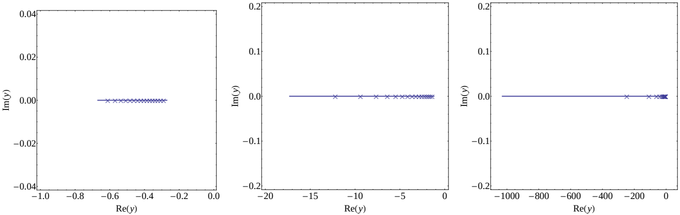

FIGURE: Roots for the ground state (a) $g = 1/10$, (b) $g = 1$, and (c) $g = 10$.

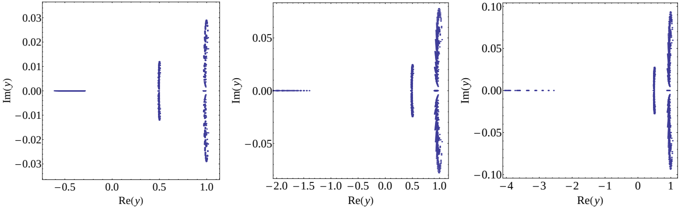

FIGURE: (a) $g = 1/10$, (b) $g = 1$, (c) $g = 10$.

$$(z^4-\gamma z^3+\eta z^2)Q''+\Big(-\frac{\eta}{2G}+\frac{1}{2}\gamma\eta L+z\Big(2\eta+\frac{\gamma}{2G}-\frac{(\gamma^2+2\eta)L}{2}-2\eta M\Big)$$
$$+\Big(-2\gamma-\frac{1}{2G}+2\gamma M\Big)z^2+(2-2M)z^3\Big)Q'$$
$$-(\beta_2 z^2+\beta_1 z+\beta_0)Q=0$$

$$\beta_2=-\left((M-1)M\right), \quad \beta_1=-\left(\gamma M+\frac{M}{2G}-\gamma M^2\right),$$
$$\beta_0=-\left(\frac{E}{2G}+\frac{\gamma L}{4}-\eta M-\frac{\gamma M}{2G}+\frac{1}{2}(\gamma-\eta)LM+\eta M^2\right).$$

- We choose $\varepsilon_2=1,\ \varepsilon_1=1/2,\ L=64,\ M=32.$
- The the ground-state roots form an arc and collapse at the origin at the critical point $g=\frac{2}{3}$

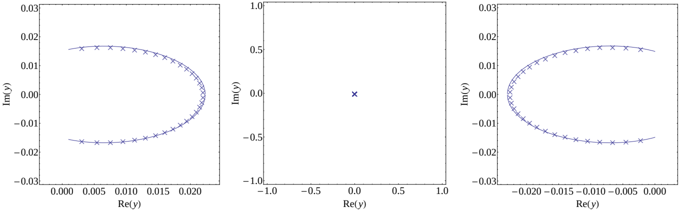

FIGURE: Roots for the ground state (a) $g = 49/75$, (b) $g = 2/3$, and (c) $g = 51/75$.

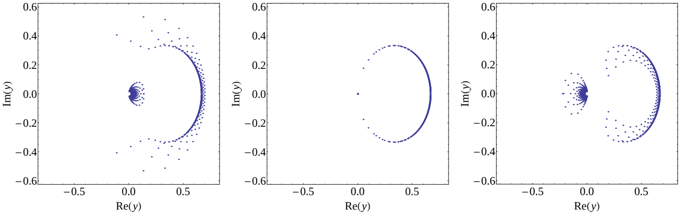

FIGURE: (a) $g = 49/75$, (b) $g = 2/3$, and (c) $g = 51/75$.

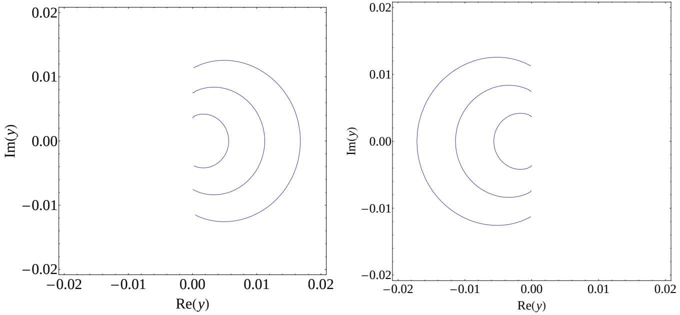

FIGURE: Theoretical curves for the large-L limit of the degenerate, two-level extended d + id-wave pairing model with $\varepsilon_2 = 1$, and $\varepsilon_1 = 1/2$, $x = lim_{L\to\infty} M/L = 1/2$: (a) From left to right g = 203/300, g = 202/300, g = 201/300, (b) From left to right g = 199/300, g = 198/300, g = 197/300. The limiting behaviour indicates that the curve contracts to a point at the origin when g = 2/3.

Critical points

- Four ground-state phase transition points associated with changes in the topology of the root distribution curve
- The behaviour of these curves and the ground-state roots of the ground state can differ greatly
- At the transiton point for the extended $d + id$-wave and the RG line of the p+ip-wave pairing the roots of all excited states cluster on common curves.

Table: Behaviour of the ground-state roots in a finite-sized system, and the distribution curves in the continuum limit, for ground-state phase transition points

Model	# roots at origin	Behavior of the curve curve
s	Nil	Closed/open transition
$p + ip$ (MR)	All	Open/closed transition
$p + ip$ (RG)	Nil	Closed curve collapse
Extended $d + id$	All	Open curve collapse/revival

Conclusion

- The method is reliable and robust. We also made a comparison between the continuum limit and the approach based on generalized Heine-Stieltjes and Van Vleck polynomials.

- We were able to observe the interesting behavior of the excited roots for the new extended d+id model

- In future : Application to other types of integrable systems or other BCS model
  -Birrell, Isaac and Links (2012) : Variational approach of quantum inverse scattering method
  -Links, Zhou, Gould and McKenzie (2002) : so(5) pairing Hamiltonian and proton-neutron interaction

- Faribault, Calabrese and Caux (2009,2010) : Quench