Appendix A

Propagation formulas for traces

$<< H^p >>^{(m_1,m_2,m_3)}$

Given Ω number of sp orbitals each with spin $\mathbf{s} = 1$, the number of sp states are $N = 3\Omega$. Now arrange these sp states in such a way that the first Ω states have $m_{\mathbf{s}} = 1$ (these are labeled $\alpha = 1$ states), the next Ω states have $m_{\mathbf{s}} = 0$ (labeled $\alpha = 2$ states) and the remaining Ω having $m_{\mathbf{s}} = -1$ (labeled $\alpha = 3$ states) so that a state $|r\rangle = |i = r, m_{\mathbf{s}} = 1\rangle$ for $r \leq \Omega$, for $\Omega < r \leq 2\Omega$, $|r\rangle = |i = r - \Omega, m_{\mathbf{s}} = 0\rangle$ and for $r > 2\Omega$, $|r\rangle = |i = r - 2\Omega, m_{\mathbf{s}} = -1\rangle$. To proceed further, the two-body Hamiltonian defined by $V^{s=0,1,2}_{i_1 j_1 k_1 \ell_1}(2)$ matrix elements is converted into the $|i, m_{\mathbf{s}} = 0, \pm 1\rangle$ basis by changing to $V_{ijkl}(2)$, where $H = 1/4 \sum_{ijkl}^{N=3\Omega} V_{ijkl}(2)\, A_i A_j B_k B_l$. Here $A(B)$ are the boson creation(destruction) operators. Given two-body matrix elements in $V_{ijkl}(2)$ form, it is possible to write propagation formulas, in configuration space $\widetilde{m} \equiv (m_1, m_2, m_3)$, for $\langle H \rangle^{\widetilde{m}}$ and $\langle H^2 \rangle^{\widetilde{m}}$ for each member of BEGOE(2)-$S1$. Note that m_1, m_2 and m_3 are number of bosons in the unitary orbits with $\alpha = 1$, 2 and 3 respectively and $m = m_1 + m_2 + m_3$. The propagation formula for energy centroid is given by,

$$\langle H \rangle^{\widetilde{m}} = \sum_{\alpha}^{3} w_{\alpha\alpha} \frac{m_\alpha (m_\alpha - 1)}{2} + \sum_{\alpha<\beta}^{3} w_{\alpha\beta}\, m_\alpha m_\beta \; . \tag{A-1}$$

Here, $w_{\alpha\beta}$ are the average two particle matrix elements for the two particles in orbits α and β and they are given by

$$w_{\alpha\beta} = \sum_{i\in\alpha, j\in\beta}^{N} \frac{V_{ijij}}{\Omega(\Omega+\delta_{\alpha\beta})} \ . \tag{A-2}$$

The spectral variance is can be written as

$$\left\langle H^2 \right\rangle^{\widetilde{m}} = \left[\left\langle H \right\rangle^{\widetilde{m}}\right]^2 + \left\langle [H(\nu=1)]^2 \right\rangle^{\widetilde{m}} + \left\langle [H(\nu=2)]^2) \right\rangle^{\widetilde{m}} \ . \tag{A-3}$$

Propagation formulas for the variances generated by the irreducible $\nu = 1$ and $\nu = 2$ parts can be written as,

$$\left\langle [H(\nu=1)]^2 \right\rangle^{\widetilde{m}} = \sum_{\alpha\beta} \left\{ \frac{m_\alpha}{\Omega} + \frac{m_\alpha(m_\alpha - \delta_{\alpha\beta})}{\Omega(\Omega+\delta_{\alpha\beta})} \right\} \sum_{i\in\alpha, j\in\beta} \left(\varepsilon_{ij}^{\alpha\beta}\right)^2 \tag{A-4}$$

and

$$\left\langle [H(\nu=2)]^2 \right\rangle^{\widetilde{m}} = \sum_{\alpha\beta\gamma\eta} \{ \frac{m_\alpha(m_\beta - \delta_{\alpha\beta})}{4\Omega(\Omega+\delta_{\alpha\beta})} + \frac{m_\alpha(m_\beta - \delta_{\alpha\beta})(m_\gamma - \delta_{\gamma\alpha} - \delta_{\gamma\beta})}{2\Omega(\Omega+\delta_{\alpha\beta})(\Omega+\delta_{\gamma\alpha}+\delta_{\gamma\beta}))}$$

$$+ \frac{m_\alpha(m_\beta - \delta_{\alpha\beta})(m_\gamma - \delta_{\gamma\alpha} - \delta_{\gamma\beta})(m_\eta - \delta_{\eta\alpha} - \delta_{\eta\beta} - \delta_{\eta\gamma})}{4\Omega(\Omega+\delta_{\alpha\beta})(\Omega+\delta_{\gamma\alpha}+\delta_{\gamma\beta})(\Omega+\delta_{\eta\alpha}+\delta_{\eta\beta}+\delta_{\eta\gamma})} \} \sum_{i\in\alpha, j\in\beta, k\in\gamma, l\in\eta} \left(V_{ijkl}^{\nu=2}\right)^2 \ . \tag{A-5}$$

The induced single particle energies $\varepsilon_{ij}^{\alpha\beta}$ in Eq. (A-4) are given by $\varepsilon_{ij}^{\alpha\beta} = \sum_\beta \xi_{ij}^{\alpha\beta} \ (m_\beta - \delta_{\alpha,\beta})$ where $\xi_{ij}^{\alpha\beta} = \sum_k V_{ikjk}^{\nu=1+2}/(\Omega + 2\delta_{\alpha\beta})$. The $\nu = 1{+}2$ part of $V(2)$ with respect to the $\widetilde{m}$'s is defined by $V_{ijkl}^{\nu=1+2} = V_{ijkl} - \delta_{ik}\ \delta_{jl}\ (1 + \delta_{ij})\ \underset{i\in\alpha, j\in\beta}{w_{\alpha\beta}}$. Similarly, the $\nu = 2$ part with respect to the $\widetilde{m}$'s is defined by $V_{ijkl}^{\nu=2} = V_{ijkl}^{\nu=1+2} - \underset{j,l\in\alpha; i,k\in\beta}{\delta_{ik}\xi_{jl}^{\alpha\beta}} - \underset{i,k\in\alpha; j,l\in\beta}{\delta_{jl}\xi_{ik}^{\alpha\beta}} - \underset{j,k\in\alpha; i,l\in\beta}{\delta_{il}\xi_{jk}^{\alpha\beta}} - \underset{i,l\in\alpha; j,k\in\beta}{\delta_{jk}\xi_{il}^{\alpha\beta}}$ and these appear in Eq. (A-5).

Appendix B

Pairing algebras for BEGOE(1+2)-$S1$

$SO(\Omega) - SU(3)$ pairing

Following the results given in [66, 78, 89] it is easy to identify the $\Omega(\Omega-1)/2$ number of generators $U(i,j)$, $i<j$ of $SO(\Omega)$ in $U(3\Omega) \supset [U(\Omega) \supset SO(\Omega)] \otimes [SU(3) \supset SO(3)]$,

$$\begin{aligned} &U(i,j) = \sqrt{\alpha(i,j)}\ [g(i,j) + \alpha(i,j)\, g(j,i)]\ , \quad i<j\ ; \\ &|\alpha(i,j)|^2 = 1, \quad \alpha(i,j) = \alpha(j,i), \quad \alpha(i,j)\alpha(j,k) = -\alpha(i,k)\ . \end{aligned} \tag{B-1}$$

Note that $g(i,j)$ are defined in Eq. (4.3.3). The quadratic Casimir invariant of $SO(\Omega)$ is,

$$\hat{C}_2(SO(\Omega)) = \sum_{i<j} U(i,j) \cdot U(j,i)\ . \tag{B-2}$$

Applying Eq. (B-1) now gives,

$$\begin{aligned} \hat{C}_2(SO(\Omega)) &= \sum_{i<j} \alpha(i,j)\,[g(i,j)\cdot g(i,j) + g(j,i)\cdot g(j,i) + 2\alpha(i,j)\, g(i,j) g(j,i)] \\ &= \sum_{i\neq j} g(i,j)\cdot g(j,i) + \sum_{i\neq j} \alpha(i,j)\, g(i,j)\cdot g(i,j) \\ &= \hat{C}_2(U(\Omega)) - \sum_{i,j} \beta_i\beta_j\, g(i,j)\cdot g(i,j)\ ; \\ \beta_i\beta_j &= -\alpha(i,j), \text{ for } i\neq j, \quad |\beta_i|^2 = 1\ . \end{aligned} \tag{B-3}$$

Here we have introduced β_is and the $\alpha(i,j)$ are defined in Eq. (B-1). Now defining the pairing operator $\mathcal{P}^k_q$, $k = 0, 2$ as

$$\mathcal{P}^k_q = \sum_i \beta_i \left(b^\dagger_{i;1} b^\dagger_{i;1} \right)^k_q \; ; \quad k = 0, 2 \tag{B-4}$$

it is easy to see that,

$$\begin{aligned} H_{\mathcal{P}} = \sum_{k=0,2;q} \mathcal{P}^k_q \left(\mathcal{P}^k_q \right)^\dagger &= \hat{C}_2(U(\Omega)) - \hat{C}_2(SO(\Omega)) - \hat{n} \\ &= \frac{2}{3}\hat{C}_2(SU(3)) - \hat{C}_2(SO(\Omega)) - (\Omega - 4)\hat{n} + \frac{\hat{n}^2}{3} \; . \end{aligned} \tag{B-5}$$

Thus the pairing Hamiltonian in the $U(3\Omega) \supset [U(\Omega) \supset SO(\Omega)] \otimes [SU(3) \supset SO(3)]$ algebra is a sum of $k = 0$ and 2 pairs and it is simply related to the $SO(\Omega)$ and $SU(3)$ algebras. It is useful to note that the two-particle matrix elements of the pairing Hamiltonian $H_{\mathcal{P}}$ are $V^{s=0}_{iijj} = 1$, $V^{s=2}_{iijj} = 1$ and all other matrix elements being zero.

It is possible to enumerate the irreps $[\boldsymbol{\omega}]$ of $SO(\Omega)$ given a $U(\Omega)$ (equivalently $SU(3)$) irrep $\{f\}$ for a given m using the methods given in [89, 123] and for some special $\{f\}$ we can also write formulas [66, 81]. Firstly, as $\{f\}$ is three rowed, the irrep $[\boldsymbol{\omega}]$ will be maximum three rowed. Then $[\boldsymbol{\omega}] = [\omega_1, \omega_2, \omega_3]$. For symmetric irreps $\{m\}$, we have the simple result,

$$\{m\} \to [\omega], \quad \omega = m, m-2, \ldots, 0 \quad \text{or} \quad 1 \; . \tag{B-6}$$

Reduction formulas for the two row irreps $\{f_1, f_2\} \to [\omega_1, \omega_2]$ and similarly for the three row irreps $\{f_1, f_2, f_3\} \to [\omega_1, \omega_2, \omega_3]$ will be complicated and they are not discussed here. As an example, we show in Table the $SO(\Omega)$ irreps contained in all $U(\Omega)$ irreps for $m = 6$ with $\Omega \geq 4$. Given the $[\omega_1, \omega_2, \omega_3]$, the eigenvalues of $\hat{C}_2(SO(\Omega))$ are given by

$$\left\langle \hat{C}_2(SO(\Omega)) \right\rangle^{[\omega_1,\omega_2,\omega_3]} = \omega_1(\omega_1 + \Omega - 2) + \omega_2(\omega_2 + \Omega - 4) + \omega_3(\omega_3 + \Omega - 6) \; . \tag{B-7}$$

Eqs. (B-5), (B-7) and (4.3.7) will give $\langle H_{\mathcal{P}} \rangle^{\{f_1,f_2,f_3\},[\omega_1,\omega_2,\omega_3]}$. It is useful to mention that, for $\Omega \geq 6$, $\omega = \omega_1 + \omega_2 + \omega_3$ is the seniority quantum number (see also Section VB). Finally, for the $U(\Omega) \supset SO(\Omega)$, the complimentary pairing algebra is the non-compact $sp(6)$ algebra generated by the 21 operators $\mathcal{P}^k_q$, $\left(\mathcal{P}^k_q\right)^\dagger$, h^1_q, h^2_q and $\hat{n}$. This complicated algebra will be discussed elsewhere; for a recent review on complimentary algebras see [124].

Table B-1: $U(\Omega) \supset SO(\Omega)$ reductions for $\Omega \geq 4$. In the table, $[\omega]^2$ implies that the irrep $[\omega]$ appears twice in the reduction.

$\{f\}$	Ω	$[\omega]$
$\{6\}$	$\Omega \geq 4$	$[6], [4], [2], [0]$
$\{5,1\}$	$\Omega \geq 4$	$[1,1], [2], [3,1], [4], [5,1]$
$\{4,2\}$	$\Omega \geq 4$	$[0], [2]^2, [2,2], [3,1], [4], [4,2]$
$\{4,1,1\}$	$\Omega \geq 6$	$[1,1], [2,1,1], [3,1], [4,1,1]$
	$\Omega = 4$	$[1,1], [2], [3,1], [4]$
	$\Omega = 5$	$[1,1], [2,1], [3,1], [4,1]$
$\{3,3\}$	$\Omega \geq 4$	$[1,1], [3,1], [3,3]$
$\{3,2,1\}$	$\Omega \geq 6$	$[1,1], [2], [2,1,1], [2,2], [3,1], [3,2,1]$
	$\Omega = 4$	$[1,1], [2]^2, [2,2], [3,1]$
	$\Omega = 5$	$[1,1], [2], [2,1], [2,2], [3,1], [3,2]$
$\{2,2,2\}$	$\Omega \geq 6$	$[0], [2], [2,2], [2,2,2]$
	$\Omega = 4$	$[0], [2]$
	$\Omega = 5$	$[0], [2], [2,2]$

Before going further, it is useful to mention that the Majorana operator $(\hat{M})$ that changes the space labels (i,j) in a two-particle space without changing the spin labels $m_{\mathbf{s}}$ is related in a simple manner to $\hat{C}_2(U(3))$. Denoting the spin labels by $\alpha, \beta, \ldots$, we have

$$\hat{M} = \sum_{i,j;\alpha,\beta} b^\dagger_{j,\alpha} b^\dagger_{i,\beta} \left(b^\dagger_{i,\alpha} b^\dagger_{j,\beta}\right)^\dagger = \hat{C}_2(U(3)) - 3\hat{n} \; . \tag{B-8}$$

Also the relation $\hat{S}^2 = \frac{4}{3}\hat{C}_2(SU(3)) - 2h^2 \cdot h^2$ from Section III shows that the $\hat{S}^2$ operator can be generated by a combination of the Majorana operator

and the quadrupole-quadrupole operator $h^2 \cdot h^2$.

$SO(3\Omega)$ pairing

Second pairing algebra follows from the recognition that $U(3\Omega)$ admits $SO(3\Omega)$ subalgebra, also the pairing here is generated by $k = 0$ pairs $b_i^\dagger \cdot b_i^\dagger$ alone, which will be seen ahead. Following the results in [78] the generators of $SO(3\Omega)$ are easy to identify and they are,

$$\begin{aligned}
&u_q^{k=1}(i,i)\ ; \quad i = 1, 2, \ldots, \Omega\ , \\
&V_q^k(i,j) = \sqrt{(-1)^k \alpha(i,j)}\ \left[u_q^k(i,j) + \alpha(i,j)\,(-1)^k\ u_q^k(j,i)\right]\ , \quad i < j\ ; \\
&|\alpha(i,j)|^2 = 1, \quad \alpha(i,j) = \alpha(j,i), \quad \alpha(i,j)\alpha(j,k) = -\alpha(i,k)\ .
\end{aligned} \tag{B-9}$$

The operators u_q^k are defined by Eq. (4.3.1). Carrying out angular momentum algebra the following relation between the quadratic Casimir invariants $\hat{C}_2(SO(3\Omega))$ and $\hat{C}_2(U(3\Omega))$, of $SO(\Omega)$ and $U(3\Omega)$), can be established using Eqs. (B-9),

$$\begin{aligned}
&\hat{C}_2(SO(3\Omega)) = 2\sum_i u^1(i,i)\cdot u^1(i,i) + \sum_{i<j;k} V^k(i,j)\cdot V^k(i,j) \\
&= \hat{C}_2(U(3\Omega)) - \sum_{i,k}(-1)^k u^k(i,i)\cdot u^k(i,i) + \sum_{i\neq j;k}(-1)^k \alpha(i,j) u^k(i,j)\cdot u^k(i,j)\ .
\end{aligned} \tag{B-10}$$

Introducing the pairing operator P_+,

$$P_+ = \sum_i \gamma_i\, P_+(i) = \frac{1}{2}\sum_i \gamma_i\, b_{i;1}^\dagger \cdot b_{i;1}^\dagger\ , \quad P_- = (P_+)^\dagger \tag{B-11}$$

we can prove the following relationship between $\hat{C}_2(SO(3\Omega))$ and the pairing Hamiltonian $H_P = 4P_+P_-$,

$$\begin{aligned}
4\,H_P = 4P_+P_- &= -\hat{n} + \hat{C}_2(U(3\Omega)) - \hat{C}_2(SO(3\Omega)) \\
&= \hat{n}(\hat{n} + 3\Omega - 2) - \hat{C}_2(SO(3\Omega))\ ; \\
\gamma_i\gamma_j &= -\alpha(i,j),\ \text{for}\ \ i \neq j, \quad |\gamma_i|^2 = 1\ .
\end{aligned} \tag{B-12}$$

The $\beta \leftrightarrow \alpha$ relation is needed for the correspondence between H_P and $\hat{C}_2(SO(3\Omega))$. Important point now being that the three operators P_+, P_- and $P_0 = (\Omega+\hat{n})/2$ will form a $SU(1,1)$ algebra complimentary to $SO(3\Omega)$. Thus the $SO(3\Omega)$ pairing is much simpler. With $U(3\Omega))$ irreps being $\{m\}$, the $SO(3\Omega)$ irreps are labeled by the seniority quantum number ω where,

$$\omega = m, m-2, \ldots, 0 \ \text{ or } \ 1 \ . \tag{B-13}$$

and H_P eigenvalues are

$$\langle H_P \rangle^{m,\omega} = \frac{1}{4}(m-\omega)(m+\omega+3\Omega-2) \ . \tag{B-14}$$

The two particle matrix elements of H_P are simply $V_{\bar{i}ij\bar{j}}^{s=0} = 1$ and all other matrix elements are zero. Let us mention that to obtain complete classification of states we need irrep reductions for $SO(3\Omega) \supset SO(\Omega) \otimes SO(3)$ and this will be discussed in future.

Appendix C

Hamiltonian for lattice chains of interacting half-spins

For a one dimensional finite chain of interacting spins-1/2 the number of lattice sites is given by L. For these L lattice sites, assigned are some up-spins and down-spins which interact with one another. An up-spin is denoted by $|\uparrow\rangle$ or equivalently by the vector $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$, whereas a down-spin is denoted by $|\downarrow\rangle$ or by $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$. The up-spin as mentioned in Chapter 6 acts as an excitation which is to be propagated throughout the chain. The Hamiltonian for such a finite chain of interacting spins-1/2 is given as follows [109]:

$$H = \sum_{n=1}^{L} \omega_n S_n^z + \varepsilon S_d^z + \sum_{n=1}^{L-1} J \ \hat{S}_n \ \hat{S}_{n+1} \tag{C-1}$$

In the construction of Hamiltonian here the spin operators $S_n^{x,y,z}$ are used which have contribution from the Pauli's matrices ($\sigma_n^{x,y,z}$) where x, y, z denote the three components in X, Y, Z directions respectively and n represents the number of lattice site. Here, J is value of interaction strength between nearest neighboring sites. It has three components J_x, J_y and J_z oriented in the X, Y and Z direction respectively. $S_n^{x,y,z} = \sigma_n^{x,y,z}/2$ are the

spin operators at site n and $\sigma_n^{x,y,z}$ are the Pauli's matrices which are given by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} ; \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} ; \sigma_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

For the present study, $\hbar$ is set as 1. The first two terms in equation C-1 explains the Zeeman splitting for each spin as determined by the static magnetic field in z-direction as stated above. Here ω_n is the energy splitting which is supposed to be equal for every site except for one, the so called defect site. This is because, here the magnetic field slight higher comparatively and hence a factor ε adds to the splitting term and makes it $\omega + \varepsilon$. If the value of defect strength (ε) is zero, then the chain is considered clean. Here, the excitation is propagated throughout the chain, represented by the last term in equation C-1. Moreover, for the chain described by equation (C-1), the z component of the total spin $\sum_{n=1}^{L} S_n^z$ is conserved, so the states with same number of excitations are coupled. To avoid degeneracy found in the spectrum of a closed chain(with periodic boundary conditions) we here consider open chains so that an excitation at site 1 moves up to the $(L-1)$ site and the momentum is not conserved. Further we shall separately study the structure of Hamiltonian for the two Heisenberg models (XXX and XXZ) referred in Chapter 6.

Heisenberg's XXX model

This is an isotropic 1D chain of interacting spins-1/2. One can write the Hamiltonian for this model using the above equation C-1. The last term may be expanded as follows:

$$\sum_{n=1}^{L-1} J \ \hat{S}_n \ \hat{S}_{n+1} = \sum_{n=1}^{L-1} J(S_n^x \ S_{n+1}^x + S_n^y \ S_{n+1}^y + S_n^z \ S_{n+1}^z) \qquad \text{(C-2)}$$

Hence the final Hamiltonian for XXX Hamiltonian is:

$$H = \sum_{n=1}^{L} \omega_n S_n^z + \varepsilon S_d^z + \sum_{n=1}^{L-1} J(S_n^x\ S_{n+1}^x + S_n^y\ S_{n+1}^y + S_n^z\ S_{n+1}^z) \qquad \text{(C-3)}$$

Here all the three components of the interaction term have the same strength i.e. $J = J_x = J_y = J_z$, hence isotropic. The term $(S_n^x\ S_{n+1}^x + S_n^y\ S_{n+1}^y)$ is called the flip-flop term and it contributes to the off-diagonal elements of the Hamiltonian matrix, whereas the $(S_n^z\ S_{n+1}^z)$ term is known as the Ising term relating to the diagonal part of the matrix. The dimensionality of this Hamiltonian matrix can be calculated from a very simple relation. If for L number of lattice sites there be $L/2$ number of excitations (up-spins) and the rest being down-spins, then dimensionality is given by the expression,

$$D = \frac{L!}{(L/2)!(L - L/2)!} \qquad \text{(C-4)}$$

For e.g. in the present case we choose $L = 14$ number of lattice sites and thus $L/2 = 7$ excitations, thus the dimensionality of the system Hamiltonian comes out to be 3432.

Heisenberg's XXZ model

This is an anisotropic chain based on the Heisenberg's XXZ model. Again here we use the equation C-1 for the construction of Hamiltonian for this chain. The basic difference between this and the precious model is just the strength of the interaction. The Hamiltonian is expressed as:

$$H = \sum_{n=1}^{L} \omega_n S_n^z + \varepsilon S_d^z + \sum_{n=1}^{L-1} [J_{xy}(S_n^x\ S_{n+1}^x + S_n^y\ S_{n+1}^y) + J_z(S_n^z\ S_{n+1}^z)] \qquad \text{(C-5)}$$

Here, the three components of the interaction strength J are not equal but they are in a relation $J_x = J_y \neq J_z$ (J_x and J_y are commonly denoted as J_{xy}). The first two terms are the same as they are in equation C-1, whereas

the nearest neighbor interaction is represented by the last term. Again here, the flip-flop term which contributes to the off-diagonal elements of the Hamiltonian matrix is given as $(S_n^x\ S_{n+1}^x + S_n^y\ S_{n+1}^y)$ and the term $(S_n^z\ S_{n+1}^z)$ represents the Ising part which contributes to the diagonal matrix elements. Also, here we modify the criterion of choosing the number of excitation according to [71] and choose subspaces filled with $L/3$ up-spins which takes care of the condition that $S^z \neq 0$. For these $L/3$ number of excitations to be distributed on L lattice sites, the dimensionality is given by,

$$D = \frac{L!}{(L/3)!(L - L/3)!} \tag{C-6}$$

Hence for the present configuration of $L = 18$ lattice sites and 6 excitations, the dimensionality will be 18564.