Chapter 7

Effect of Symmetry on Quantum Transport Across Disordered Networks Connected by Many-Body Interactions

7.1 Introduction

In this chapter, we study an interesting application of the embedded random matrix ensembles with k-body interactions introduced in chapter 4. The efficient transport of particles or excitations (known as quantum efficiency) plays a very important role in understanding various open problems in the field of quantum transport. This requires the fundamental knowledge of quantum physics and non-equilibrium statistical mechanics [159]. In this chapter, our main goal is to study the role of centrosymmetry on transport efficiencies across disordered finite networks (fermionic/bosonic) modeled by embedded random-matrix ensembles of k-body interactions.

In last about half a century, with the emergence of quantum physics, the world witnessed evolutionary miniaturization of electronic devices from macro to micro to nano scale. This in-turn, resulted in a rapidly developing field of nanoscience and nanotechnology, due to the significant properties that appear because of novel quantum effects at nano-scale. The physics of macro devices cannot explain these novel quantum effects in nano-scale devices. For this purpose one must consider quantum transport, tunnelling and interference effects, and discreteness of electron charge. A very important as well as a challenging part of this field is quantum efficiency, which addresses the efficient transport of particles or excitations across complex quantum systems. It plays a crucial role in designing nano-scale devices with increased efficiency [159]. Recently, in the field of condensed matter physics, quantum transport is studied in one dimensional nano wires(which may have spintronics applications), Quantum Anomalous Hall (QAH) phase with ultracold atoms, graphene and carbon nanotubes [160], quantum dots [161], solar cells [162], superconducting nanocircuits [163, 164], nano-scale MOSFET devices [160, 165–167],etc. Quantum efficiency also plays a vital role in understanding the state transfer between quantum processors in quantum computers [168, 169], quantum key distribution [170], teleportation, photosynthetic biomolecules [171–175], the Fenna-Matthews-Olson (FMO) light-harvesting biomolecules [176], quantum optics, etc. The design of highly efficient quantum devices is still an open area of research and this motivates us to construct quantum systems, having high quantum efficiency.

So far, various approaches have been developed to study quantum transport in complex quantum systems. Some of these approaches include the Landauer formula and Buttiker probes, Boltzmann transport models, scattering approach [177], non-equilibrium Green's function (NEGF) formalism, Density Functional Theory (DFT) [178], etc. NEGF formalism was first introduced by Martin and Schwinger and later developed by Kadanoff, Baym and Keldysh [159] and is now the most frequently used formalism. These systems can also be modeled by a disordered random network of nodes and links [179, 180]. A lot of progress has been achieved for quantum transport in open systems using random scattering matrix approach. Topological superconductors, chaotic cavities [181], metallic carbon nanotubes [182], quantum dot and disordered wire ([183] and references therein) have been studied using this approach. On the other hand, for quantum transport in closed systems, random Hamiltonian approach i.e. random matrix theory is used. This is studied for disordered quantum dots [184]. However, quantum transport in closed systems remains barely studied. These studies suggest that RMT is well positioned to explore the universal aspects of quantum transport. Using a disordered network of d sites and employing GOE for the Hamiltonian, it was shown in [179] that highly efficient quantum transport is possible for the Hamiltonian with centrosymmetry and a dominant doublet spectral structure. Recently, it has been shown by Ortega et. al. that the transport efficiency can be enhanced just with centrosymmetry when GOE is replaced by EGOE(k) [34, 76–78]. These works show that efficient quantum transport is achieved when the Hamiltonian preserves centrosymmetry.

In one dimensional nanowires, graphene, quantum dots, solar cells, nano-scale devices, etc. fermions play a very important role. Also, in QAH phase with ultracold atoms and superconducting nanocircuits bosons play an important role. This motivated us to study quantum transport across disordered (fermionic/bosonic) networks. In all these applications, it is crucial to transport a quantum state as well as map it with other constituents of the device. This results in transport of particles/excitations among these nano-scale devices. This has been studied in the past in the case of quantum dots [185, 186] and ultracold atoms trapped in optical lattices [187].

In this chapter we study the role of centrosymmetry on transport efficiencies across disordered finite networks of m (fermions/bosons) distributed in N sp states, connected via k-body interactions and modeled by EE of k-body interactions. For fermions these ensembles are symbolized as EGOE(k) and for bosons they are symbolized as BEGOE(k). We have used three different ensembles that include many-body interactions for both fermionic and bosonic networks. It is seen that presence of centrosymmetry in these networks enhances quantum efficiency. However, in the absence of centrosymmetry (or non-centrosymmetric structure of the Hamiltonian), quantum transport is not enhanced. Quantum transport across non-centrosymmetric structures is studied by various groups using various other approaches as well. Some of these include the very recent works on magnetic and electrical transport in non-centrosymmetric Nd_7Ni_2Pd [188] and charge transport in non-centrosymmetric superconductors [189]. This chapter is organized as follows. We begin with the definition of centrosymmetry and understand how we can impose centrosymmetry in EE with k-body interactions and hence the construction of centrosymmetric EGOE(k). The next section describes transport efficiency and Perfect State Transfer (PST). Moving ahead, the next section presents the results of the best efficiencies. Finally, the last section gives conclusions. This chapter is based on [190].

7.2 Embedded Ensembles for Disordered Networks: Introducing Centrosymmetry

In chapter 4, we have described the construction of EGOE(k) and BEGOE(k). In this chapter we model the fermionic and bosonic disordered networks using EGOE(k) and BEGOE(k) respectively to study the role of centrosymmetry in quantum transport across them. The nodes of the network are the basis states of the Hilbert space and the correlations among matrix elements are related to the links of the network.

Now let us define centrosymmetry. A symmetric $d \times d$ matrix H is defined as centrosymmetric if it commutes with the exchange matrix J i.e. $JH = HJ$. The exchange matrix J is defined by $J_{i,j} = \delta_{i,d-i+1}$, $\delta_{i,j}$ is the Kronecker delta. The exchange matrix is simply an antidiagonal identity matrix [191]. In the present work the matrix H is constructed using EGOEs with and without centrosymmetry. Centrosymmetry can be introduced to the k-body EE using the following approaches given in [76]: (i) at the one-particle level, which is the core for the definition of the k and m particle Hilbert spaces, (ii) at the k-body level, where the actual (random) parameters of the embedded ensembles are set, or (iii) at the m-body level, which defines the dynamics. The Hamiltonian of realistic systems consist of a mean field one-body term in addition to the two-body (residual) interaction (i.e. $H = H_{k=1} + H_{k=2}$). Hence, it will be inappropriate to define a specific transformation for each term separately. Therefore, we will impose it in the one-particle space and see how it propagates to k-body and m-body space. Centrosymmetry imposed in the one-particle space is defined by $J_1 \left|j\right\rangle = \left|N-j+1\right\rangle$, for $j = 1, 2, ..., N$. It's matrix representation in the one-body basis is precisely the exchange matrix. Now, let us see how it is imposed in fermionic systems. For simplicity, first let's consider a system of two fermions. In this case, we can define $J_2\psi^{\dagger}_{2;j_1,j_2} = J_1 a^{\dagger}_{j_1} J_1 a^{\dagger}_{j_2} = -\psi^{\dagger}_{2;N-j_2+1,N-j_1+1}$. The global minus sign due to anticommutation relations, can be neglected as the indices are arranged in increasing order. Generalizing the above equation for k-particles, we get

$$J_k\psi^{\dagger}_{k;j_1,\ldots,j_k} = \prod_{n=1}^{k} J_1 a^{\dagger}_{j_n} = \psi^{\dagger}_{k;N-j_k+1,\ldots,N-j_1+1} \tag{7.1}$$

Now for a system of two bosons, we define $J_2\chi^{\dagger}_{2;j_1,j_2} = N_\alpha J_1 b^{\dagger}_{j_1} J_1 b^{\dagger}_{j_2} = \chi^{\dagger}_{2;N-j_2+1,N-j_1+1}$. Here N_α is the normalization constant. Generalizing this for k-particles

$$J_k\chi^{\dagger}_{k;j_1,\ldots,j_k} = N_\alpha \prod_{s=1}^{k} J_1 b^{\dagger}_{j_s} = \chi^{\dagger}_{k;N-j_k+1,\ldots,N-j_1+1} \tag{7.2}$$

The matrix J_k in Eqs. (7.1) and (7.2), is not an exchange matrix, i.e., the matrix with ones in the secondary diagonal and zeros elsewhere. This follows from the possible existence of more than one state that is mapped by J_k onto itself; in this case, we shall say that J_k is a partial exchange matrix [76].

In the present work, we study transport efficiencies in a small fermionic as well as bosonic network by employing three models: (i) EGOE(k) (and BEGOE(k)) without centrosymmetry, (ii) EGOE(k) (and BEGOE(k)) with centrosymmetry present in both k as well as m particle space [denoted by csEGOE(k) (and csBEGOE(k))] and (iii) EGOE(k) (and BEGOE(k)) with centrosymmetry present in k-particle space [denoted by EGOE(k-cs) (and BEGOE(k-cs))]. In csEGOE(k) (and csBEGOE(k)) case, centrosymmetry is imposed in the one particle space and then it is propagated to k and m particle spaces [76–78] while in EGOE(k-cs) (and BEGOE(k-cs)), centrosymmetry is imposed in k-particle spaces and then it is propagated to m-particle spaces using the many-particle Hilbert space geometry. In the first case (i.e. csEGOE(k) (and csBEGOE(k)), the final Hamiltonian preserves centrosymmetric structure while it is not preserved in the latter case (i.e. EGOE(k-cs) (and BEGOE(k-cs)). Now let us examine the matrix structure of Hamiltonian when centrosymmetry is imposed in BEGOE(k). Fig. 7.1 illustrates the structure of H matrix for the cases csBEGOE(k) and BEGOE(k-cs). One can see that structure of H matrix is symmetric about both the diagonals which demonstrates that centrosymmetric structure is preserved. For $N = 2$, csBEGOE(k) and BEGOE(k-cs) are identical. Therefore centrosymmetric structure is preserved in BEGOE(k-cs) also.

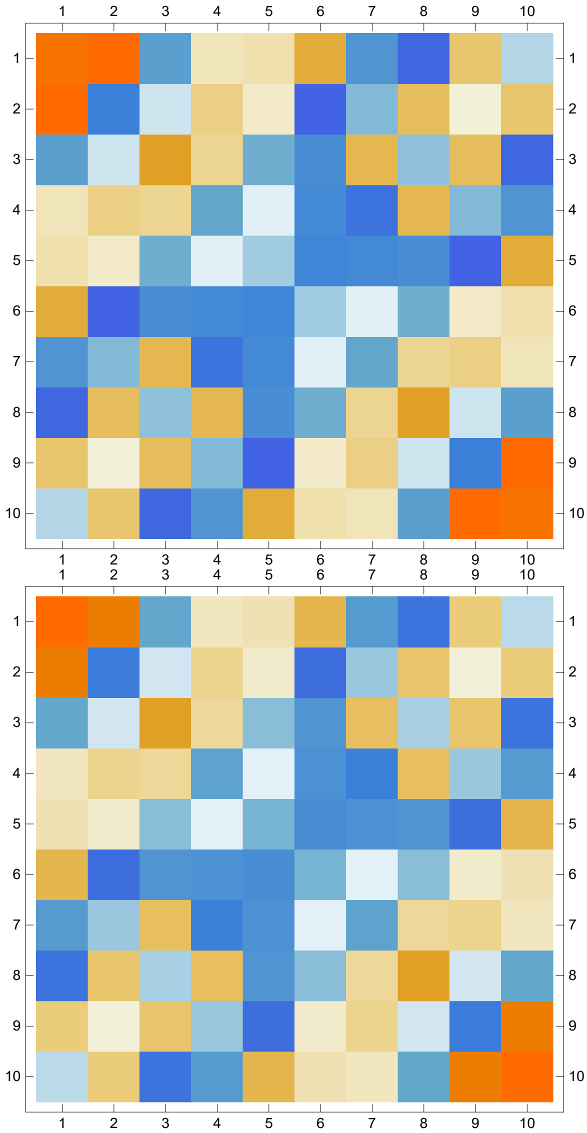

Figure 7.1: Illustration of structure of H matrix for (i) csBEGOE(k) (above) and (ii) BEGOE(k-cs) (below) by distributing $m = 9$ bosons in $N = 2$ sp states. The total number of basis states being $d = 10$. Note that csBEGOE(k) and BEGOE(k-cs) are identical for $N = 2$.

7.3 Transport Efficiency and Perfect State Transfer (PST)

In realistic complex quantum systems, only a limited degree of control is available. Hence, it is very important to find out under what conditions near-to-perfect transport between two states of a small disordered interacting quantum system can be improved [179]. Such systems can be modeled by a disordered random network of nodes and links [179,180].

Initially, the network is prepared in state $|in\rangle = |n_i\rangle$ and an excitation is introduced. Here, during the state transfer, only the state $|in\rangle$ is controlled and there is no control over it's dynamics. As the network evolves unitarily, the excitation propagates to the state $|out\rangle = |n_f\rangle$. Note that the initial $|n_i\rangle$ and final $|n_f\rangle$ excitations are localized on the nodes of the network. Then, the maximum transition probability achieved among these states within a time interval $[0, T]$ is termed as the transport efficiency, which is quantitatively defined as [179, 192].

$$P_{i,f} = max_{[0,T]} | \langle n_f | U(t) | n_i \rangle |^2 \tag{7.3}$$

Here, we choose T such that maximum is reached in Eq. (7.3) and hence $\hbar = 1$. Here, $U(t)$ is the unitary quantum evolution associated with the Hamiltonian H of the network. The value of $P_{i,f}$ is always between 0 and 1, higher the value of $P_{i,f}$, better is the transfer. The network is said to have perfect state transfer (PST) when $P_{i,f} = 1$ [169]. In other words, the fidelity is unity and hence the system is considered as efficient. In [179] the time scale T was defined separately for each random matrix realization, essentially by the direct coupling matrix element between the $|n_i\rangle$ and $|n_f\rangle$ states. But in the case of EE, such matrix element may be identically zero. Hence, we use the same time scale for all realizations of the ensemble. In general, random disorder adds a constraint to transport due to Anderson localization. Hence, it is necessary to identify structural elements which provide efficient quantum transport in the presence of disorder [78]. Realistic systems preserve additional symmetries (in addition to particle number m) like angular momentum, parity, spin-isospin SU(4) symmetry, and so on [31]. Various works suggest that additional strong correlations arise when realistic systems preserve centrosymmetry, which in turn remarkably enhances the state transport across such systems [179, 193–195]. In addition to centrosymmetry, decoherence can also enhance efficiency in disordered networks [78]. However, there is ongoing debate on the relation between coherence and efficiency [192]. In the next section we present results of normalized distributions and mean of the probability distributions of the best efficiencies for both fermionic and bosonic networks.

7.4 Effect of Centrosymmetry on Quantum Transport

7.4.1 Transport Efficiency in Disordered Fermionic Networks

We begin with the study of role of centrosymmetry in quantum transport across fermionic networks. Consider a network generated by distributing $m = 1$ to $N - 1$

fermions in $N = 6$ sp states. We vary the body rank of interaction k from 1 to m. Here, it is important to consider all body ranks of interaction as in bio-molecules, correlations among many particles can be present. The distribution of best efficiencies P is computed for each member of the ensemble as the distribution of efficiencies of the ensemble is rather broad. We have used an ensemble of 2000 members in each calculation. We first calculate the normalized distributions of the best efficiencies P as a function of interaction rank k and the normalized distributions are shown in Fig.7.2. The red histograms correspond to EGOE(k), the black histograms correspond to csEGOE(k) and the green histograms correspond to EGOE(k-cs). One can observe that the transport efficiencies for EGOE(k) (network with lack of centrosymmetry) is less than 80% for various values of m and k. However, it can be seen that below and at half-filling only for $k = m = 1$ the transport efficiency reaches above 90% while above half filling, for $m = 5$ the transport efficiencies roughly reach 80%. Now, let us see what happens when we introduce centrosymmetry across these networks i.e. with csEGOE(k). In this case, there is PST for $k = 1$ for all values of m, especially when the number of fermions m is odd. Also, when k or m are odd, the Hamiltonian preserves centrosymmetric structure, as a result efficiency is enhanced. For example, for $k = 3$ and $m = 5$, transport efficiency is 95 %. Also, above half filling, we obtain best efficiencies. These results are in good agreement with the previous study [76]. Further, it is very important to know, how efficient the transport will be in such quantum network if centrosymmetry is imposed in k-particle space i.e. using EGOE(k-cs). In this case also, PST is achieved for $k = 1$ for all values of m, especially when the number of fermions m is odd. Also, when k or m are odd, efficiency is enhanced. For example, for $k = 3$ and $m = 5$, transport efficiency is 90%. In addition to this, we have also calculated the average value (mean) of best efficiencies P. Fig. 7.3 represents the mean of probability distributions of the best efficiencies $\langle P \rangle$ as a function of body rank of interaction k for (i) EGOE(k) (red open squares) (ii) csEGOE(k) (black open squares) and (iii) EGOE(k-cs) (green open squares). The open squares represent mean of best efficiencies P and vertical bars represent widths of the distributions. It is evident from the results shown in Fig.7.2 that the presence of centrosymmetry enhances transport efficiencies. We have also carried out similar analysis for $N = 7$. The normalized distributions of the best efficiencies P as a function of interaction rank k are computed and the normalized distributions are shown in Fig.7.4, which demonstrate the same trend as in the case of $N = 6$. Also results of the mean of best efficiencies P are shown in Fig. 7.5. Here also we observe same trend as in the case of $N = 6$.

However, it is important to note that in this approach, the dimension of k-particle space also plays a crucial role. If the dimension of k-particle space is high, it decreases the transport efficiency across these networks. We demonstrate this with the help of the following example. We consider $N = 8$ and vary the body rank of interaction k from

1 to $m = 7$. The results are shown in Fig. 7.6. Here improvement in the efficiency is not observed. This suggests that even if we have odd values of k or m and above half filling, PST may not be achieved if the dimension of k-particle space is high. This proves that these studies are suitable only for phenomena and devices at nano-scale having low dimensions.

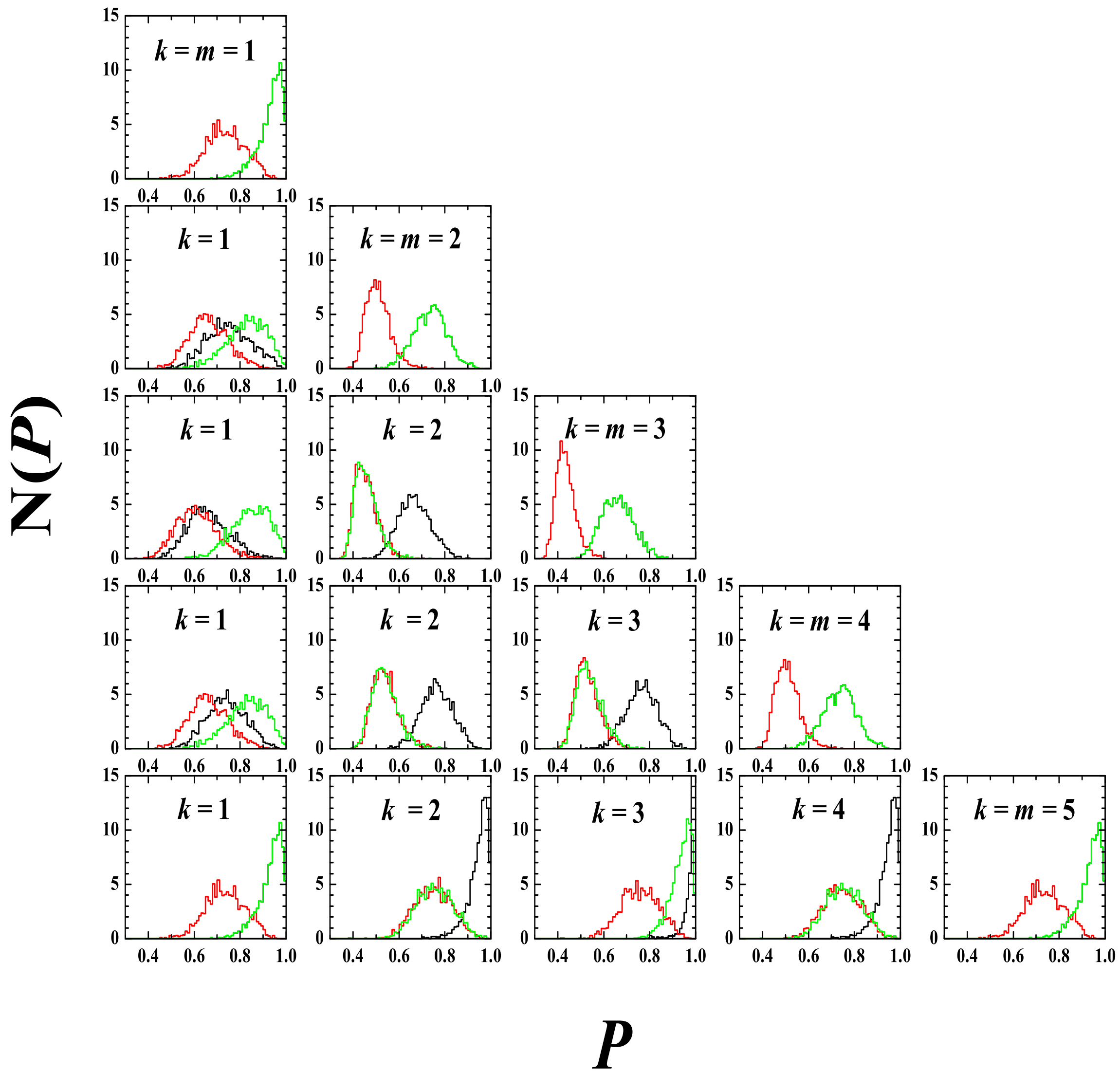

Figure 7.2: Normalized distributions of the best efficiencies P for a 2000 member (i) EGOE(k) (red histogram) (ii) csEGOE(k) (black histogram) and (iii) EGOE(k-cs) (green histogram) with $N = 6$ and m is varied from 1 to 5.

7.4.2 Transport Efficiency in Disordered Bosonic Networks

Now, we study the role of centrosymmetry in quantum transport across bosonic networks. It is important to note that with bosons, it is possible to have dense network, a situation not feasible for fermions due to applicability of Pauli's exclusion principle. First,

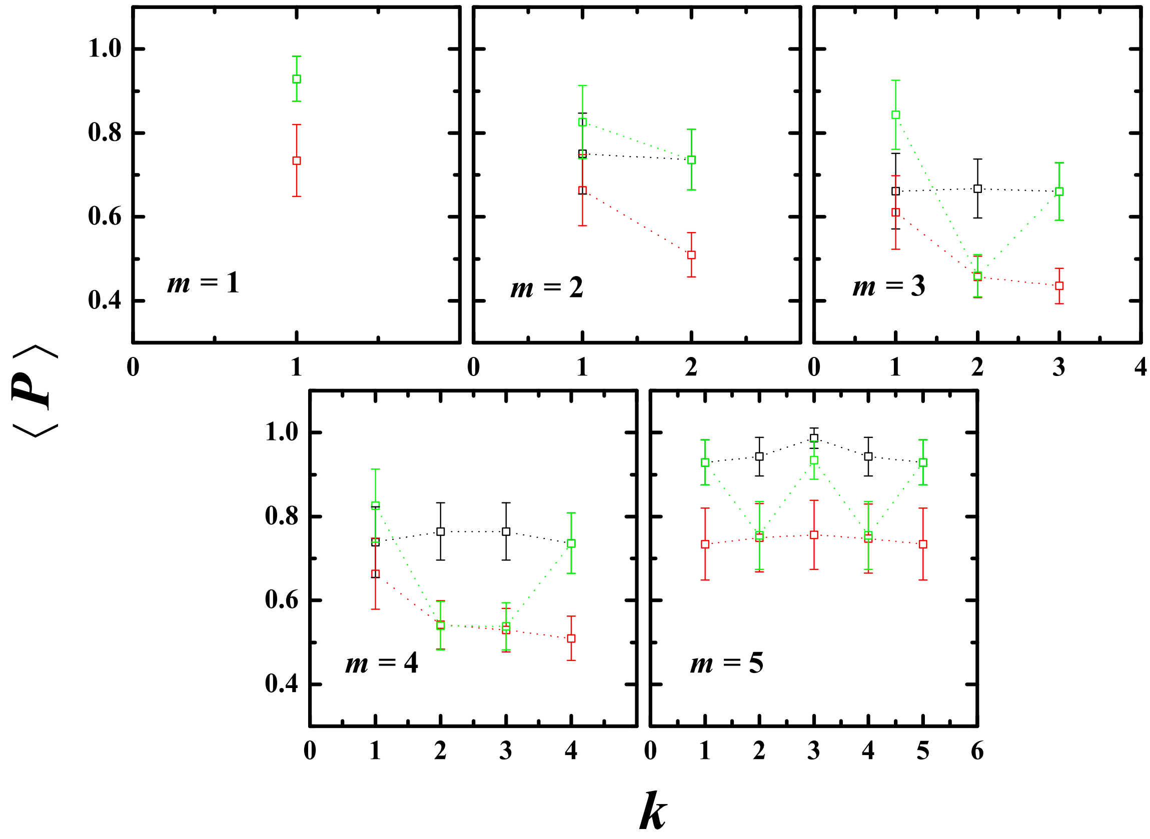

Figure 7.3: Mean of the probability distributions of the best efficiencies $\langle P\rangle$ (denoted by open squares) and corresponding widths of the distributions (denoted by vertical bars) for a 2000 member (i) EGOE(k) (red squares), (ii) csEGOE(k) (black squares) and (iii) EGOE(k -cs) (green squares) as a function of body rank of interaction k . Here $N = 6$ sp states and m is varied from 1 to 5. Here dotted line is just to guide the eye. Refer text for more details.

we consider a network generated by basis states obtained by distributing $m = 9$ bosons in $N = 2$ sp states. The total number of basis states are $d = 10$ in this case and we represent the network Hamiltonian by a 2000 member (i) BEGOE(k), (ii) csBEGOE(k) and (iii) BEGOE(k -cs). For a two-level ($N = 2$), csBEGOE(k) and BEGOE(k -cs) are identical by construction [76]. The normalized distributions of the best efficiencies P are calculated by varying the interaction rank k and the normalized distributions are presented in Fig.7.7. The red histograms correspond to BEGOE(k) and the black histograms correspond to csBEGOE(k). The results shown in Fig.7.7 clearly demonstrate that the presence of centrosymmetry enriches transport efficiencies. We also calculate the best efficiencies P about the mean of each member of ensemble. The results are presented in Fig. 7.8. Open squares represent the average value of probability distributions of the best efficiencies P of each member of ensemble, calculated as a function of interaction rank k . The vertical bars represent the width of probability distributions of the best efficiencies P about the mean of each member of ensemble. The red open squares correspond to BEGOE(k) while the results for csBEGOE(k) are represented by black open squares. It is evident from the results

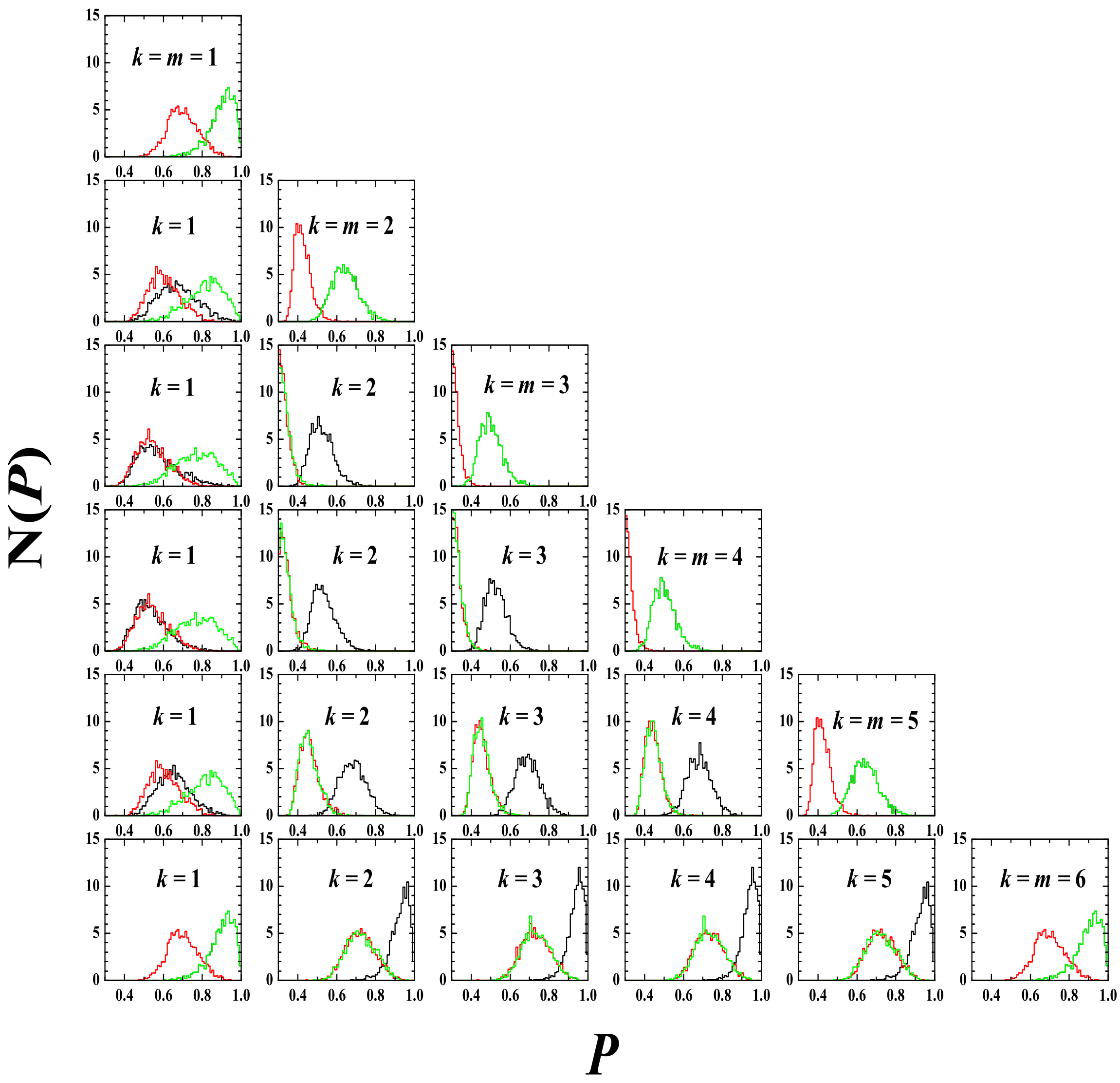

Figure 7.4: Same as Fig. 7.2 but for network with $N = 7$ and m is varied from 1 to 6. Refer text for more details.

shown in Fig.7.8 that the presence of centrosymmetry enhances transport efficiencies and these results are in good agreement with those obtained in [76].

Moving further, we consider a network generated by basis states obtained by distributing $m = 6$ bosons in $N = 3$ sp states. The dimensionality of the network is $d = 28$ in this case. Here, we varied the number of bosons m from 1 to 6. The results of normalized distributions of the best efficiencies P are shown in Fig.7.9. In the figure, the number of bosons m is same along the rows while the value of k is same along the columns. It can be seen that the transport efficiency for BEGOE(k) (in absence of centrosymmetry) is less than 80% for almost all the cases. With BEGOE(k-cs), there is a marginal improvement for all $k > 1$ as centrosymmetry structure is lost in m-particle space although it is present in k-particle space. While on the other hand, in presence of centrosymmetry, with csBEGOE(k), one can observe that the efficiency is around 90% for $k \leq 3$. This clearly demonstrates that the presence of centrosymmetry enhances the transport efficiency. Note that for $k = m$, BEGOE(k -cs) and csBEGOE(k) are identical and they are GOE with centrosymmetry. For csBEGOE(k), there is a PST for $m = 3$ and $k \leq 3$. It is interesting to note that for $k = m = 1$, BEGOE(k -cs) gives PST for $m = 1 - 6$. The lack of PST for $N = 3$ levels beyond $m = 3$ and $k \leq 3$ in comparison to $N = 2$ example can be attributed to a systematic appearance of doublets in the spectrum for $N = 2$ [169]. The mean of probability distributions of the best efficiencies $\langle P \rangle$ as a function of body rank of interaction k are shown in Fig.7.10. These results also demonstrate that the presence of centrosymmetry enhances the transport efficiency.

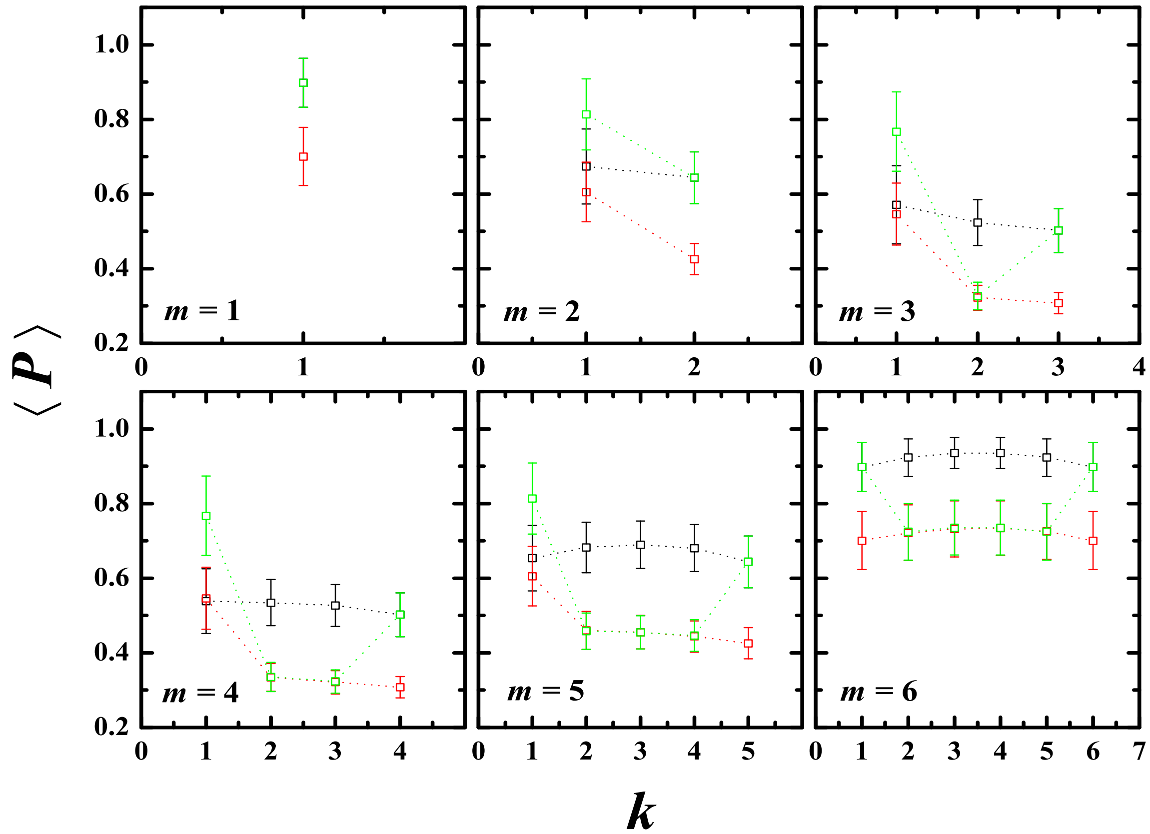

Figure 7.5: Same as Fig. 7.3 but for network with $N = 7$ and m is varied from 1 to 6. Refer text for more details.

These results show the importance of presence of centrosymmetry in optimal transport across disordered fermionic and bosonic networks. The absence of which leads to inefficient quantum transport.

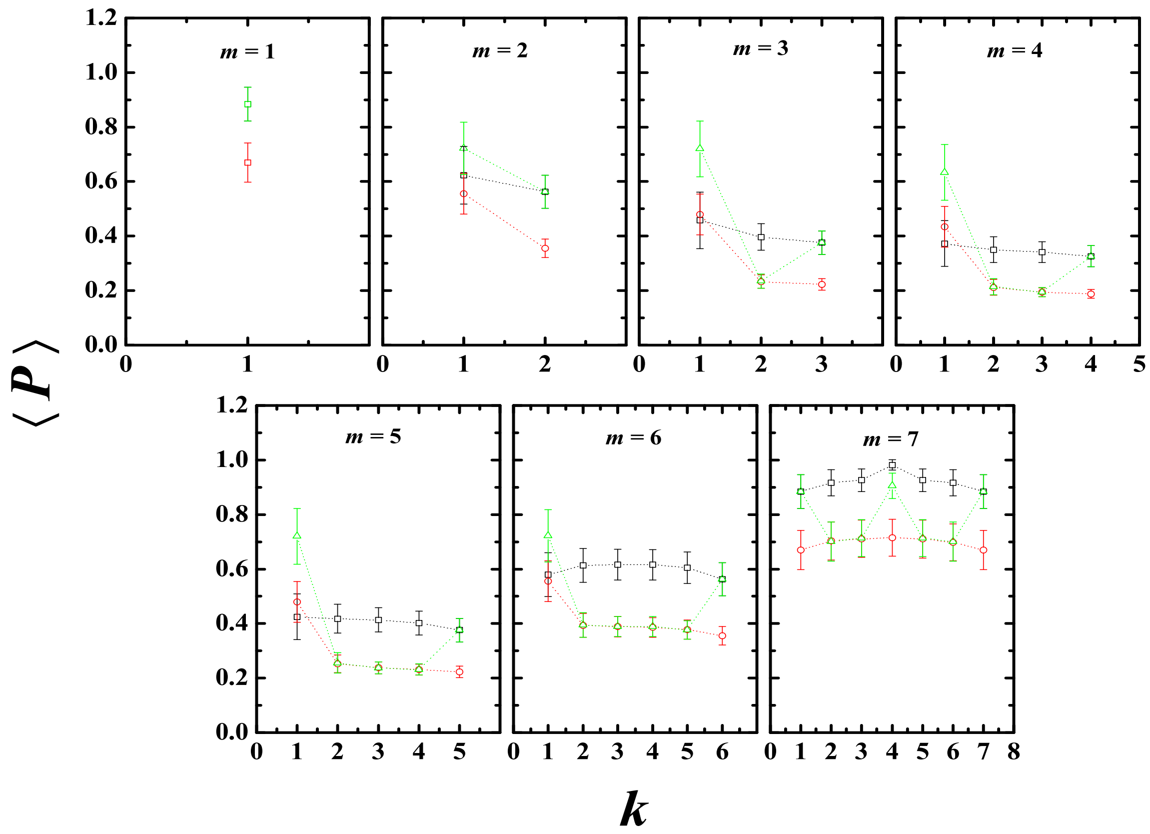

Figure 7.6: Same as Fig. 7.3 but for network with $N = 8$ and m is varied from 1 to 7. Refer text for more details.

7.5 Conclusions

In this chapter, we have studied transport efficiency across disordered fermionic and bosonic networks modeled by k-body embedded Gaussian ensembles EGOE(k) (or BEGOE(k)) for fermions (or bosons) in absence and presence of centrosymmetry. We found that the presence of centrosymmetry in m-particle space is responsible for the enhancement of transport efficiency in a small network and results are in good agreement with [76]. Further, we also verified that the centrosymmetry structure is essentially needed in both, k-particle as well as in m-particle space, to enhance quantum efficiency. Following the results presented in this chapter, it is possible to design networks with good efficiency even in presence of certain many-body random perturbations. However, it is observed that the dimension of k-particle space also plays a crucial role in this approach. If the dimension of k-particle space is high, it hinders the transport efficiency across these networks, making these studies suitable only at nano-scale (i.e. low dimensions).

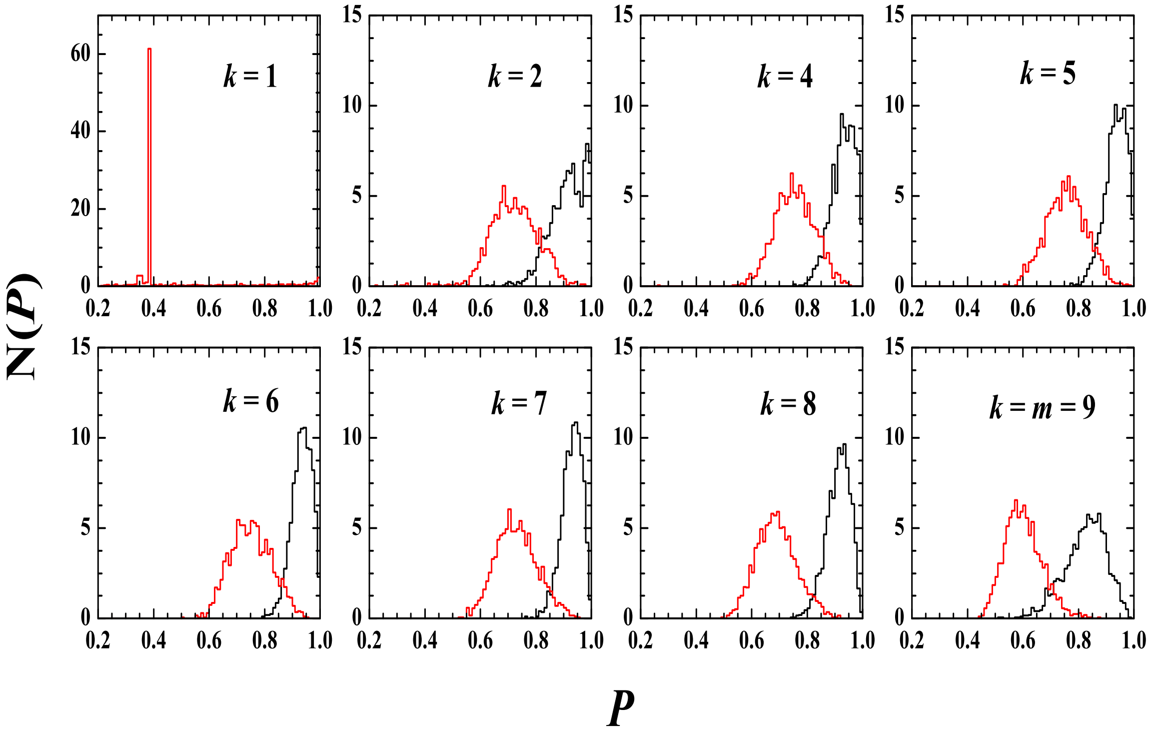

Figure 7.7: Normalized distributions of the best efficiencies P for a 2000 member (i) BEGOE(k) (red histogram) and (ii) csBEGOE(k) (black histogram) with $N = 2$ and $m = 9$ as a function of interaction rank k. Note that, BEGOE(k-cs) and csBEGOE(k) are identical for $N = 2$. Similar results are reported in [76].

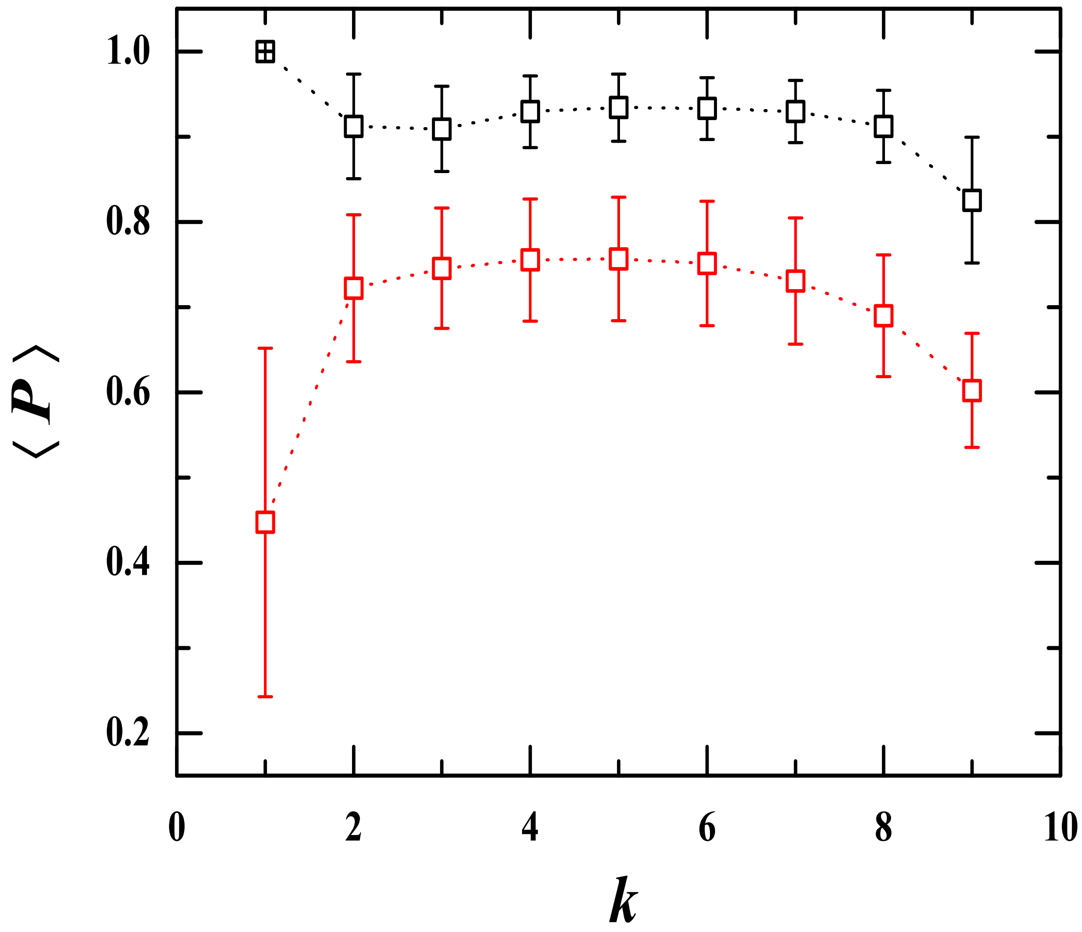

Figure 7.8: Mean of the probability distributions of the best efficiencies $\langle P \rangle$ (denoted by open squares) and corresponding widths of the distributions (denoted by vertical bars) for a 2000 member (i) BEGOE(k) (red squares) and (ii) csBEGOE(k) (black squares) with $N = 2$ sp states and $m = 9$ as a function of body rank of interaction k . Here dotted line is just to guide the eye. Note that, BEGOE(k -cs) and csBEGOE(k) are identical for $N = 2$. Similar results are reported in [76]. Refer text for more details.

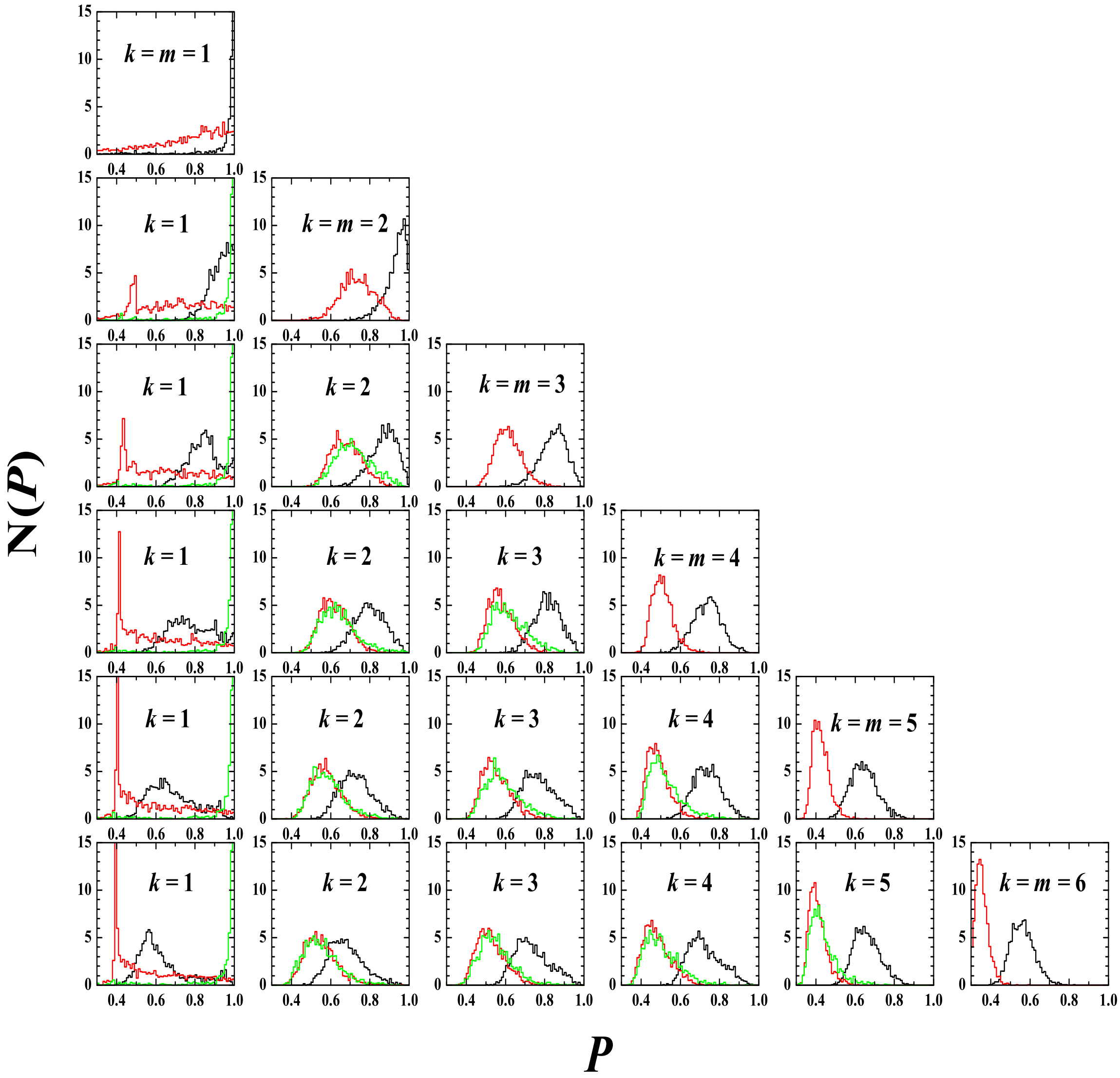

Figure 7.9: Normalized distributions of the best efficiencies P for a 2000 member (i) BEGOE(k) (red histogram), (ii) BEGOE(k -cs) (green histogram) and (iii) csBEGOE(k) (black histogram) with $N = 3$ and $m = 6$ as a function of m and interaction rank k. Rows have the same particle number m and columns have the same k value. Note that for $k = m$, results for BEGOE(k -cs) and csBEGOE(k) are identical.

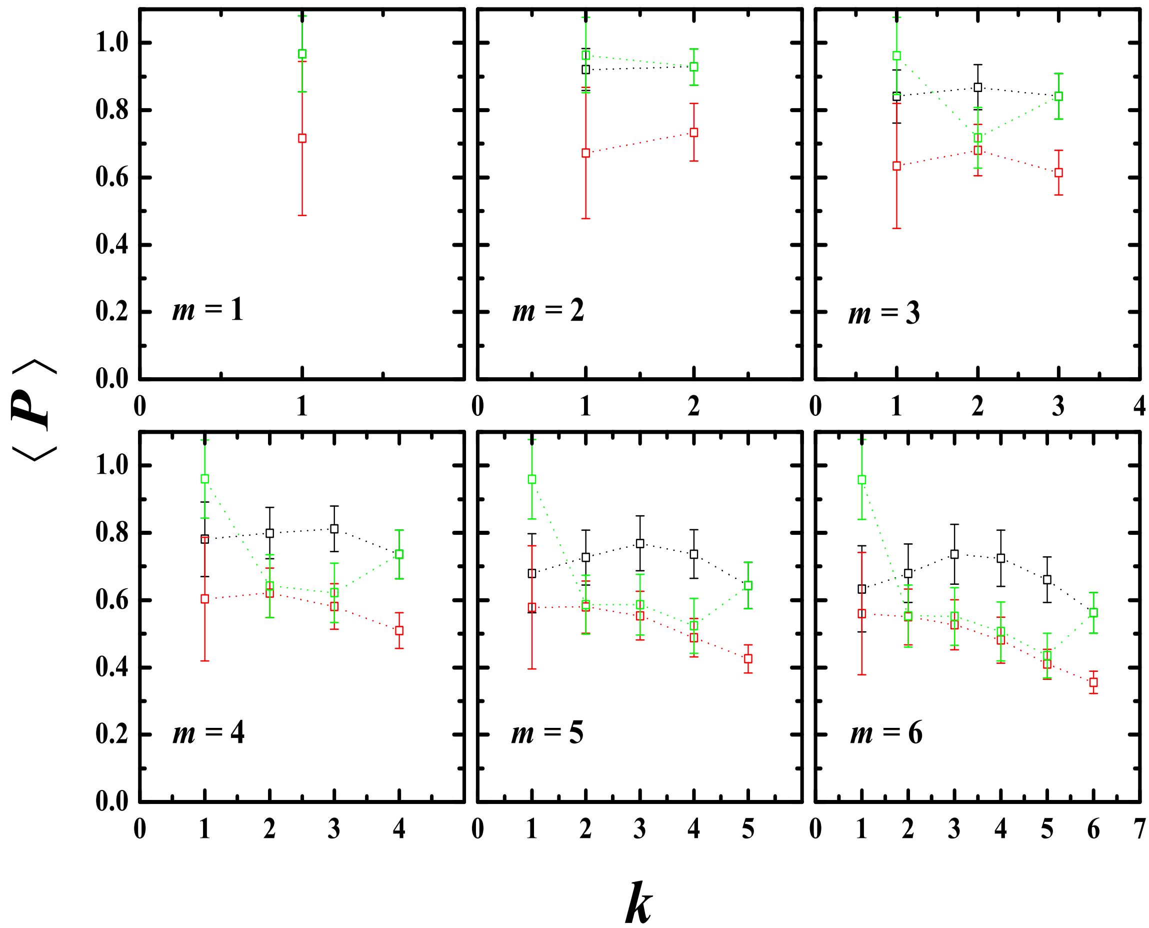

Figure 7.10: Same as Fig. 7.8 but for a 2000 member (i) BEGOE(k) (red squares), (ii) csBEGOE(k) (black squares) and (iii) BEGOE(k-cs) (green squares) as a function of body rank of interaction k. Here $N = 3$ sp states and m is varied from 1 to 6. Note that for $k = m$, results for BEGOE(k-cs) and csBEGOE(k) are identical. Refer text for more details.