

**CLASSICAL AND QUANTUM STATISTICAL
MECHANICS OF PERMUTATION REPRESENTATIONS**

JONATHAN D.H. SMITH

Department of Mathematics
Iowa State University
Ames, IA 50011, USA

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Abstract

Let G be a finite group acting transitively on a set Q . Then for each natural number r , the group G has a diagonal action on the cartesian power Q^r . Exponential generating functions for the multiplicities of the irreducible characters of G in the permutation representations of G on Q^r are furnished by Gibbs canonical distributions from classical and quantum statistical mechanics. The argument of the generating functions is interpretable as a temperature. Asymptotically, almost all orbits of a faithful representation are regular. The classical concept of a class function on the group G is replaced by the quantum mechanical operator of right multiplication by the class function. In particular, right multiplication by a permutation character is interpretable as the Hamiltonian of a quantum system.

1. Introduction.

Suppose that a finite group G acts transitively on a set Q . For each natural number r , the group G then has a diagonal action on the cartesian power Q^r (5.3). This paper is concerned with the problem of specifying the decomposition of the linear permutation representation of G on Q^r as a sum of (complex) irreducible linear representations of G . For instance, the multiplicity of the trivial representation counts the number of orbits of G on Q^r . Such considerations have two immediate motivations. As part of a programme studying the analysis of variance in statistics [Sp1-8], T.P. Speed formulated his Orbit Problem [Sp9, §7] asking for a description of the orbits of the action of G on Q^r . The second motivation arises from the character theory of quasigroups [J 1-6], the extension of the character theory of groups to "non-associative groups". In this theory, the character table Ψ of a group or quasigroup Q is obtained from the eigenmatrices of the association scheme (Q, Γ) given by the diagonal action of the multiplication group G of Q on Q^2 [J1], (4.4), (4.7). For a group Q with character table Ψ , the tensor square $\Psi \otimes \Psi$ is the character table of Q^2 . For a general quasigroup Q , this need no longer be true. However, in [J4] the concept of a "superscheme" was introduced, an extension of the concept of an association scheme to relations of arbitrary length. An interpretation of the tensor square of the character table of Q was given in terms of the action of the Bose-Mesner algebra of (Q, Γ) on the relations of length 3 in the superscheme (Q, Γ^*) of G on Q [J4, Theorem

7.1]. Later, it was shown that every superscheme (Q, Γ^*) arises as the set of orbits of a permutation group G on Q acting diagonally on the powers Q^r of Q [Sm1, Th. 4.4]. Thus a good description of the diagonal actions of a group G on the powers Q^r is essential for understanding superschemes.

An earlier paper [Sm3] used the incidence algebra of the subgroup lattice of G over the rational Burnside algebra of G to describe the decomposition of Q^r into G -orbits. In the current paper, the focus is on complex linear representations. The key theme is to use concepts from classical and quantum physics to address the problem. Section 2 gives a quick summary of the relevant aspects of classical statistical mechanics, while Section 3 does the same for quantum mechanics and quantum statistical mechanics. In the fourth section, a quantum mechanical framework for the character theory of a finite group G is established. The Hilbert space \mathcal{H} of class functions on G is taken as the underlying Hilbert space of a quantum mechanical system. The space \mathcal{H} has two orthonormal bases: one, X , given by the irreducible characters of G , and the other, Δ , by the (normalized) characteristic functions of the conjugacy classes of G . The unitary change-of-basis matrix from Δ to X is a normalized version (4.4) of the character table of G , symmetrically mediating the eigenmatrices of the association scheme on G given by the action of the multiplication group of G on G^2 (4.7). The “classical” concept of a class function θ on G is replaced by the “quantum” concept of the operator $R(\theta)$, right multiplication by θ in the commutative algebra of class functions on G under componentwise operations. If θ is real-valued, e.g. the character of a permutation representation, then $R(\theta)$ is an observable in the sense of quantum mechanics.

The final two sections use statistical mechanics ideas to describe the action of G on Q^r . In the fifth section, the exponential generating function for the number of orbits of G on Q^r is exhibited as a classical partition function (Theorem 5.1). In combinatorics, the argument of a generating function is considered as a purely formal “place-holding” device. The statistical-mechanical approach enables one to interpret the argument of the exponential generating function as a physical quantity, the temperature (2.7). Theorem 5.1 may also be viewed as an “inverse Laplace transform” of Molien’s Theorem [Mo] on the ring of invariants of G on $\mathbb{C}Q$ (Remark 5.2). As a consequence of Theorem 5.1, it

is shown that almost every class of a superscheme is a regular orbit. Section 6 uses the quantum mechanical approach from the fourth section. The permutation character π of G on Q yields an operator $R(\pi)$ that may be interpreted as the Hamiltonian of a quantum system. The corresponding Gibbs canonical state of quantum statistical mechanics then yields exponential generating functions for the multiplicities of the various irreducible characters of G in the permutation representations of G on the powers Q^r (Theorem 6.1). The arguments of the generating functions again admit a physical interpretation as temperatures.

2. Classical statistical mechanics.

Suppose that a (classical) physical system has a finite number s of possible (macro-) states, corresponding to energy values E_1, E_2, \dots, E_s (say in joules). The actual state of the system is unknown: all that is known is the expected value

$$(2.1) \quad E = \sum_{i=1}^s p_i E_i$$

of the energy with respect to the (unknown) probability distribution (p_1, p_2, \dots, p_s) of the states. The probability distribution satisfies the normalization

$$(2.2) \quad 1 = \sum_{i=1}^s p_i.$$

The randomness of such a probability distribution is measured by its "Shannon" or *information-theoretic entropy*

$$(2.3) \quad - \sum_{i=1}^s p_i \log p_i.$$

One's total ignorance about the system, with the unique exception of (2.1), is then expressed by assigning that probability distribution which maximizes (2.3) subject only to (2.1) and (2.2). The probability distribution is Gibbs' *canonical distribution*

$$(2.4) \quad p_i = Z(t)^{-1} \exp(tE_i)$$

with (*classical*) *partition function* or "Zustandsumme"

$$(2.5) \quad Z(t) = \sum_{i=1}^s \exp(tE_i)$$

[Gr, 3A], [Sm2]. The value E from (2.1) is recovered as

$$(2.6) \quad E = \frac{d}{dt} \log Z(t).$$

Conversely, since by (2.5) the logarithm $\log Z(t)$ of the partition function is strictly convex, each fixed value E determines a unique parameter value t via (2.6). By (2.4), the Lagrange multiplier t has dimension the reciprocal of energy. Setting

$$(2.7) \quad t = -\frac{1}{kT}$$

with k as Boltzmann's constant 1.38×10^{-23} joules per degree Kelvin, one obtains T as the temperature (in degrees Kelvin) of the system when it has energy E (in joules).

3. Quantum statistical mechanics.

A quantum mechanical system corresponds to a separable Hilbert space \mathcal{H} . An *observable* of the system corresponds to an Hermitian or self-adjoint operator $H : \mathcal{H} \rightarrow \mathcal{H}$. A *state* of the system corresponds to a non-negative Hermitian operator $\rho : \mathcal{H} \rightarrow \mathcal{H}$ of unit trace. If the system is in state ρ , and an observation H is made on the system, then the value $\text{Tr}(\rho H)$ is observed. Recall that the *trace* $\text{Tr}(A)$ of an operator A is the sum

$$(3.1) \quad \text{Tr} A = \sum_{i=1}^{\dim \mathcal{H}} \langle \varphi_i, A \varphi_i \rangle$$

for any complete orthonormal basis $(\varphi_i | 1 \leq i < 1 + \dim \mathcal{H})$ of \mathcal{H} . Technically, A is required to be "of trace class", guaranteeing the absolute convergence of (3.1). Such analytical details will be irrelevant here, where the spaces \mathcal{H} appearing actually have finite dimension. In this case, the trace of an operator in the sense of (3.1) is just the trace (sum of all diagonal entries) of its matrix with respect to an orthonormal basis of \mathcal{H} .

Example 3.1. A spinning electron, stationary at a known location, corresponds to the space \mathbb{C}_1^2 of complex (1×2) -matrices with inner product $\langle u, v \rangle = \frac{1}{2} u v^*$. The observables of spin in the x, y and z directions correspond respectively to $\hbar/2$ times the *Pauli matrices*

$$(3.2) \quad \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},$$

where \hbar is Planck's constant 1.05×10^{-34} joule-seconds. Thus if the electron is in state $\frac{1}{10} \begin{bmatrix} 6 & 2i \\ -2i & 4 \end{bmatrix}$, the observed spin in the y direction will be $\frac{\hbar}{20} \text{Tr} \left(\begin{bmatrix} 6 & 2i \\ -2i & 4 \end{bmatrix} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \right) = -2.1 \times 10^{-35}$ joule-seconds. \square

Typically, one does not know the detailed state of a system, but only the values of certain observables. Let H be the Hamiltonian of a system – the observable whose value gives the energy of the system. Suppose the state ρ is completely unknown, except that it corresponds to a definite energy value E :

$$(3.3) \quad E = \text{Tr}(\rho H).$$

This is the quantum analogue of (2.1). Indeed, if \mathcal{H} has finite dimension s and, with respect to some orthonormal basis, ρ has diagonal matrix $\text{diag}(p_1, p_2, \dots, p_s)$, while H has the diagonal matrix $\text{diag}(E_1, E_2, \dots, E_s)$, then (3.3) reduces exactly to (2.1). In the quantum case, the randomness of a state ρ is measured by its “von Neumann” or *quantum entropy*

$$(3.4) \quad -\text{Tr}(\rho \log \rho)$$

[Th, (2.2, 4)]. In a fashion analogous to the classical case, one's total ignorance about the system, with the unique exception of (3.3), is then expressed by assigning it the *Gibbs canonical state*

$$(3.5) \quad \rho = Z_q(t)^{-1} \exp(tH)$$

with (*quantum*) *partition function*

$$(3.6) \quad Z_q(t) = \text{Tr} \exp(tH)$$

[Gr, 4B] [Ma, §2-8] [Th, (2.4,5)].

4. Quantum mechanics of group characters.

Let G be a finite group of order n , with conjugacy classes $C_1 = \{1\}, C_2, \dots, C_s$ and irreducible characters $1 = \chi_1, \chi_2, \dots, \chi_s$. Let the sizes of the conjugacy classes be $n_i = |C_i|$, and the degrees of the irreducible characters be $f_i = \chi_i(1)$, for $i = 1, 2, \dots, s$. The character

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table is the $(s \times s)$ -matrix Ψ , with entries ψ_{ij} giving the value of χ_i at elements of C_j . Let \mathcal{H} be the s -dimensional complex vector space of class functions on G , equipped with the inner product

$$(4.1) \quad \langle \theta, \varphi \rangle = \frac{1}{n} \sum_{g \in G} \theta(g) \overline{\varphi(g)}.$$

Then \mathcal{H} is a separable Hilbert space with orthonormal basis $X = (\chi_1, \chi_2, \dots, \chi_s)$ [Se, Th. 2.6]. The quantum mechanical approach to group characters regards \mathcal{H} as the underlying Hilbert space of a quantum mechanical system. (For instance, the group of order 2 corresponds to the spinning electron of Example 3.1.) The orthonormal basis X for \mathcal{H} yields an orthogonal decomposition

$$(4.2) \quad \mathcal{H} = \mathcal{H}_1^X \oplus \mathcal{H}_2^X \oplus \dots \oplus \mathcal{H}_s^X$$

of \mathcal{H} . Let Π_i^X be the projection operator onto the i -th summand of (4.2). With respect to the orthonormal basis X , the operator Π_i^X has elementary matrix E^{ii} , the diagonal matrix whose only non-zero entry is a 1 in the (i, i) -position. Thus each Π_i^X is a state of the system.

For $1 \leq i \leq s$, let ϕ_i be the characteristic function of the conjugacy class C_i . Then $\Delta = \left\{ \phi_i \sqrt{n/n_i} \mid 1 \leq i \leq s \right\}$ is a second orthonormal basis for \mathcal{H} , yielding an orthogonal decomposition

$$(4.3) \quad \mathcal{H} = \mathcal{H}_1^\Delta \oplus \mathcal{H}_2^\Delta \oplus \dots \oplus \mathcal{H}_s^\Delta$$

of \mathcal{H} . Let Π_i^Δ be the projection operator onto the i -th summand of (4.3). Then each Π_i^Δ is also a state of the system, having matrix E^{ii} with respect to the orthonormal basis Δ .

Let U be the $(s \times s)$ -matrix whose (i, j) -entry is

$$(4.4) \quad U_{ij} = \psi_{ij} \sqrt{\frac{n_j}{n}}.$$

Then U is the unitary matrix changing from the orthonormal basis Δ to the orthonormal basis X . Thus if an operator A has matrices A_Δ with respect to Δ and A_X with respect to X , one has

$$(4.5) \quad A_X = U^{-1} A_\Delta U.$$

As a consequence, one obtains the useful formula

$$(4.6) \quad \text{Tr} (\Pi_i^X \Pi_j^\Delta) = |\psi_{ji}|^2 \frac{n_i}{n}$$

for the value of the observable Π_i^X on the state Π_j^Δ , or equivalently the value of the observable Π_j^Δ on the state Π_i^X .

The unitary matrix U has the symmetrical expression

$$(4.7) \quad U_{ij} = \sqrt{\frac{f_i}{nn_j}} \xi_{ji} = \sqrt{\frac{nn_j}{f_i}} \bar{\eta}_{ij}$$

in terms of the mutually inverse complex matrices $\Xi = (\xi_{ij})_{s \times s}$ and $H = (\eta_{ij})_{s \times s}$ relating the incidence matrices and the orthogonal idempotents of the association scheme (G, Γ) on G given by the action of the multiplication group $\text{Mlt } G$ [BI, Th. 2.7.2][J1,§3]. Here Ξ and nH are Delsarte's "eigenmatrices" ([De], cf. [BI, Ch. 2, (3.10)]).

Theorem 4.1. *Let θ be a real-valued class function on G , restricting to the constant θ_i on C_i . Define*

$$(4.8) \quad R(\theta) = \sum_{i=1}^s \theta_i \Pi_i^\Delta.$$

Then $R(\theta)$ is an observable of the system, taking the value θ_i on the state Π_i^Δ .

Proof. With respect to the orthonormal basis Δ , the operator $R(\theta)$ has real matrix $\text{diag} (\theta_1, \theta_2, \dots, \theta_s)$. Thus $R(\theta)$ is an observable. With respect to Δ , the state Π_i^Δ has elementary matrix E^{ii} . Thus $\text{Tr} (\Pi_i^\Delta R(\theta)) = \text{Tr} [E^{ii} \text{diag} (\theta_1, \theta_2, \dots, \theta_s)] = \theta_i$. \square

The space \mathcal{H} of complex-valued class functions on G is a commutative algebra under componentwise multiplication. One may extend the definition (4.8) to general elements θ of \mathcal{H} (although $R(\theta)$ need no longer be an observable then).

Theorem 4.2. *The map R yields an injective \mathbb{C} -algebra homomorphism*

$$(4.9) \quad R : \mathcal{H} \rightarrow \text{End } \mathcal{H}; \quad \theta \mapsto (R(\theta) : \varphi \mapsto \varphi\theta)$$

into the ring of operators on \mathcal{H} .

Proof. Since $\{\Pi_i^\Delta | 1 \leq i \leq s\}$ is a complete set of orthogonal idempotents, one has $R(\varphi\theta) = \sum_{i=1}^s \varphi_i \theta_i \Pi_i^\Delta = \left(\sum_{i=1}^s \varphi_i \Pi_i^\Delta \right) \left(\sum_{j=1}^s \theta_j \Pi_j^\Delta \right) = R(\varphi)R(\theta)$ and $R(1) = 1_{\mathcal{H}}$. Moreover, $\varphi\theta = 1R(\varphi\theta) = 1R(\varphi)R(\theta) = \varphi R(\theta)$. \square

Corollary 4.3. The (i, j) -entry of the matrix of $R(\theta)$ with respect to X is $\langle \chi_i \theta, \chi_j \rangle = \sum_{k=1}^s \langle \chi_i, \phi_k \rangle \frac{n \theta_k}{n_k} \langle \phi_k, \chi_j \rangle$. \square

Corollary 4.4. With $R(\theta)$ as in (4.4), the value of $R(\theta)$ on the state Π_1^X is the multiplicity $\langle \theta, \chi_1 \rangle$ of χ_1 in θ . \square

5. Classical partition functions count orbits.

Let G be a group of finite order n , having a permutation representation on a finite set Q yielding permutation character π . Thus for g in G , the character value $\pi(g)$ is the number of fixed points of g in Q . Consider the elements of G to be the states of a classical physical system, as in §2. Associate energy value $\pi(g)$ with the state g in G . The corresponding partition function is given by (2.5) as

$$(5.1) \quad Z(t) = \sum_{g \in G} e^{t\pi(g)}.$$

This expands as

$$(5.2) \quad Z(t) = \sum_{r=0}^{\infty} \frac{t^r}{r!} \sum_{g \in G} \pi(g)^r.$$

For each natural number r , the action of G on Q yields a *diagonal action* of G on Q^r with

$$(5.3) \quad g : Q^r \rightarrow Q^r; (q_1, \dots, q_r) \mapsto (q_1 g, \dots, q_r g)$$

for elements g of G . (In terms of universal algebra, the G -set (Q^r, G) is the r -th direct power of the G -set (Q, G) in the variety of G -sets.) The permutation representation of G on Q^r is the r -th tensor power of the permutation representation of G on Q , so the permutation character of G on Q^r is π^r (cf. [Se, §2.2]). By Burnside's Lemma [Hu, Satz V 13.4] the number of orbits of G on Q^r is the average number

$$(5.4) \quad \frac{1}{n} \sum_{g \in G} \pi(g)^r$$

of fixed points. Recall that the *exponential generating function* of a sequence (a_0, a_1, \dots) is $f(t) = \sum_{r=0}^{\infty} a_r \frac{t^r}{r!}$ [Wi, §2.3].

Theorem 5.1. *The quotient*

$$(5.5) \quad \frac{Z(t)}{Z(0)} = \exp \int_0^t E(s) ds$$

is the exponential generating function for the number of orbits of G on Q^r .

Proof. Note $Z(0) = n$, by (5.1). Then (5.2) and (5.4) show that the left hand side of (5.5) is the required exponential generating function. For the right hand side of (5.5), E as a function of s is given by (2.6) with $E(s) = \frac{d}{dt} \log Z(t)|_{t=s}$. The equality (5.5), in the form $\log Z(t) - \log Z(0) = \int_0^t E(s) ds$, follows by the Fundamental Theorem of the Calculus. \square

Remark 5.2. Suppose that G is a permutation group on Q . Extend the elements of G to automorphisms of the complex vector space $\mathbb{C}Q$ with basis Q . In invariant theory, the ordinary generating function for the number of orbits of G on Q^r appears as the Poincaré series

$$(5.6) \quad P_G(s) = \frac{1}{n} \sum_{g \in G} \det(1 - gs)^{-1}$$

the tensor algebra of

of the ring of invariants of G acting on $\mathbb{C}Q$ [Sr, Prop. 4.1.3]. Then $s^{-1}P_G(s^{-1})$ is the Laplace transform of $Z(t)/Z(0)$. \square

The (right) *regular* permutation action of G is the G -set G with actions

$$(5.7) \quad g : G \rightarrow G; x \mapsto xg$$

for g in G . The following result was proved in [Sm3] by use of Burnside ring techniques.

Corollary 5.3. *Suppose that the permutation representation of G on Q is faithful. Then for large powers r , almost every orbit of G on Q^r is regular.*

Proof. Since the permutation representation of G on Q is faithful, its kernel is $\{1\}$. Thus 1 is the only element g of G with $\pi(g) = \pi(1)$. For non-identity elements g of G , the non-negative quotient $\pi(g)/\pi(1)$ is strictly less than 1. The number of orbits of G on Q^r is

$$(5.8) \quad \frac{\pi(1)^r}{n} \sum_{g \in G} \left[\frac{\pi(g)}{\pi(1)} \right]^r.$$

For large r , all the summands in (5.8) except $[\pi(1)/\pi(1)]^r$ are small. Thus the number of orbits of G on Q^r tends to $\pi(1)^r/n$. In other words, almost every one of the $\pi(1)^r$ elements of Q^r lies in a regular orbit, the unique type of orbit of size n . \square

Corollary 5.4. *Let (Q, Γ^*) be a superscheme on a set Q . By [Sm1, Th. 4.4], there is a permutation group G acting on Q such that, for each natural number r , the set Γ^r of classes of (Q, Γ^*) of length $r + 2$ is the set of orbits of G acting diagonally on Q^{r+2} . Thus almost all classes of the superscheme are regular orbits of G . \square*

6. Quantum Gibbs states of permutation representations.

As in the previous section, let G be a group of finite order n acting on a finite set Q , with permutation character π . Let \mathcal{H} be the Hilbert space of class functions on G . As in Section 4, \mathcal{H} is considered as the underlying Hilbert space of a quantum mechanical system. By Proposition 4.1, $R(\pi)$ is an observable of the system. By Corollary 4.4, the value of $R(\pi)$ on the state Π_1^X is the number of orbits of G on Q .

Now consider the observable $R(\pi)$ to be the Hamiltonian of the quantum system. Then according to (3.5), the quantum partition function

$$(6.1) \quad Z_q(t) = \sum_{i=1}^s \frac{1}{n_i} \sum_{g \in C_i} e^{t\pi(g)}$$

given by (3.6) normalizes the observable

$$(6.2) \quad e^{tR(\pi)} = \sum_{i=1}^s \frac{1}{n_i} \sum_{g \in C_i} e^{t\pi(g)} \Pi_i^\Delta$$

to yield the Gibbs canonical state

$$(6.3) \quad \rho(t) = Z_q(t)^{-1} e^{tR(\pi)}.$$

Theorem 6.1. (i) *The value of the unnormalized Gibbs state observable $e^{tR(\pi)}$ on the state Π_1^X is the exponential generating function (5.5) for the number of orbits of G on Q^r .*

(ii) *The entries of the first row of the matrix of the unnormalized Gibbs state observable $e^{tR(\pi)}$ with respect to the orthonormal basis X of irreducible characters yield exponential*

generating functions for the multiplicities of the corresponding characters in the permutation representation of G on Q^r .

Proof. (i) Apply Corollary 4.4.

(ii) Apply Corollary 4.3, with $i = 1$. \square

Example 6.2. Consider the natural representation of the symmetric group $G = S_3$ on the set $Q = \{1, 2, 3\}$. Take C_2 to be the class of transpositions, and C_3 to be the class of 3-cycles. Take χ_2 to be the sign character and χ_3 to be the irreducible 2-dimensional character. With respect to the basis Δ , $e^{tR(\pi)}$ has diagonal matrix

$$(6.4) \quad \begin{bmatrix} e^{3t} & 0 & 0 \\ 0 & e^t & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

By Corollary 4.3, it follows that $e^{tR(\pi)}$ has matrix

$$(6.5) \quad \frac{e^{3t}}{6} \begin{bmatrix} 1 & 1 & 2 \\ 1 & 1 & 2 \\ 2 & 2 & 4 \end{bmatrix} + \frac{e^t}{2} \begin{bmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \frac{1}{3} \begin{bmatrix} 1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \end{bmatrix}$$

with respect to the basis X . One obtains the exponential generating functions

$$(6.6) \quad \frac{e^{3t}}{6} + \frac{e^t}{2} + \frac{1}{3} = 1 + 1t + 2\frac{t^2}{2!} + 5\frac{t^3}{3!} + 14\frac{t^4}{4!} + \dots$$

for the number of orbits (multiplicity of χ_1),

$$(6.7) \quad \frac{e^{3t}}{6} - \frac{e^t}{2} + \frac{1}{3} = 0 + 0t + 1\frac{t^2}{2!} + 4\frac{t^3}{3!} + 13\frac{t^4}{4!} + \dots$$

for the multiplicity of χ_2 , and

$$(6.8) \quad \frac{e^{3t}}{3} - \frac{1}{3} = 0 + 1t + 3\frac{t^2}{2!} + 9\frac{t^3}{3!} + 27\frac{t^4}{4!} + \dots$$

for the multiplicity of χ_3 in the permutation representation of S_3 on the powers of its natural representation. \square

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