

Maximal energy extraction under discrete diffusive exchange

M. J. Hay,^{1,a)} J. Schiff,² and N. J. Fisch^{1,3}

¹*Department of Astrophysical Sciences, Princeton University, Princeton, New Jersey 08544, USA*

²*Department of Mathematics, Bar-Ilan University, Ramat Gan 52900, Israel*

³*Princeton Plasma Physics Laboratory, Princeton, New Jersey 08543, USA*

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Waves propagating through a bounded plasma can rearrange the densities of states in the six-dimensional velocity-configuration phase space. Depending on the rearrangement, the wave energy can either increase or decrease, with the difference taken up by the total plasma energy. In the case where the rearrangement is diffusive, only certain plasma states can be reached. It turns out that the set of reachable states through such diffusive rearrangements has been described in very different contexts. Building upon those descriptions, and making use of the fact that the plasma energy is a linear functional of the state densities, the maximal extractable energy under diffusive rearrangement can then be addressed through linear programming. © 2015 AIP Publishing LLC.

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I. INTRODUCTION

Waves propagating through a bounded plasma can rearrange the densities of states in the six-dimensional velocity-configuration phase space. When the rearrangement is such as to cause particles to diffuse from higher energy states to lower energy states, the waves extract energy from the plasma. A particular case of this posing of the rearrangement problem is the case of alpha channeling, where the energy is deliberately extracted from the population of α -particles that are produced in a fusion reactor.¹ This energy is recovered as wave energy. In a reactor, this energy is more useful in the form of wave energy, which can be used to attain a hot-ion mode or to drive electrical current.

The rearrangements contemplated in plasma using waves are diffusive in nature, since the wave-particle mechanisms generally cannot maintain coherence, at least not for the leading way of using external rf sources to heat or drive current in plasma. However, depending on the wave frequency and wavenumber, the diffusion occurs in paths that link energy to the spatial dimensions. In the case of tokamak reactors, where α -particles are expected to be born at high energy in the plasma center, there is a natural energy inversion along the path that connects the dense phase space location at high energy in the center to the under-dense phase space location that is at low energy on the periphery. It is then only a matter of constructing the appropriate wave diffusion path to link these locations. How much energy can be released from α -particles is a matter of considerable practical interest, since if appreciable energy could be released in this manner, there then might be the opportunity to diminish substantially the cost of electricity through tokamak fusion.

A theoretical issue of academic interest, however, is the precise maximum available energy under diffusive rearrangements of phase space density when an arbitrary number of diffusion paths can be constructed.² The energy extractable under diffusion was posed recently, in fact, as one of the interesting,

outstanding problems in wave-particle physics in plasma.³ This issue also motivated to some extent approaches to other bounds on energy exchange between light and plasma, such as the extent to which bounds could be placed on the absorption of laser light at an interface.⁴ There are, to be sure, also other formulations of free energy in plasma under phase space density rearrangements. For example, respecting phase space conservation, the Gardner restacking^{5,6} represents a precisely definable free energy that can be readily calculated. This energy is an upper bound on that which can be extracted through diffusive processes. However, because the Gardner restacking is without the realistic limitation of the diffusion constraint, the free energy available under this formulation represents a rather rarefied theoretical construct, even further from practical considerations than the academic issue posed here.

The free energy under the constraint of diffusive rearrangements has one well-known textbook example: the so-called “bump-on-tail” problem. The tail of the Maxwellian distribution is imagined to have a “bump” in velocity space, so that the distribution is no longer monotonically decreasing in energy. In this case, waves can diffuse particles so as to smooth out the bump, releasing the kinetic energy, until a distribution monotonically decreasing in energy is reached. The maximum extractable energy is obvious and can be constructed from geometrical considerations; for the one-bump problem, it is just the energy change in flattening the bump. However, where there are two bumps in the velocity space, then the optimal solution would no longer be obvious at all, since it is not clear which bump should be flattened first.

More generally, what is imagined here is that diffusion paths can be constructed that link any two phase space locations in the 6D velocity-configuration space, whether or not the locations are contiguous.² The contiguous constraint can formally be realized, in any event, in the limit of vanishingly thin paths. Thus, we imagine an ensemble of discrete phase space locations, each with an initial density, and each representing a certain energy. Then, as population densities relax under diffusion, the total system energy relaxes as well. The

^{a)}hay@princeton.edu

free energy under the diffusion constraint is then defined as the maximum extractable energy, given the opportunity to diffuse particles between any two phase space locations, with any sequence of such two-location or what we might call two-state relaxations. It turns out, however, that while this pair-wise relaxation is a well-defined posing of the free energy, it has not been apparent at all how to calculate it efficiently when there are many states.

The problem thus posed in plasmas can similarly be posed with respect to stimulated emission by a set of lasers.² Consider an initially cold ensemble of two-level atoms in the ground state. Pumped by a resonant, incoherent source, each atom oscillates between the ground and excited states. (The energy levels correspond to the discrete phase space locations employed in the plasma model.) For pump durations long compared to the Rabi period, the atoms are evenly divided between the two states, a higher-entropy arrangement associated with a larger number of microstates. In a practical system of multilevel atoms, a train of pulses varying in frequency could be used to populate specific states or liberate energy stored in metastable excited states.

For a particular example,² consider an ensemble of atoms with only three energy levels, the ground state at energy ϵ_0 , the first excited state at ϵ_1 , and the second excited state at ϵ_2 . The number of atoms prepared in each state is denoted n_0^i , with $i = \{1, 2, 3\}$ identifying the energy level. The total energy can be written $W = \vec{\epsilon} \cdot \vec{n}$, where $\vec{\epsilon}$ and \vec{n} represent the energy levels and the population densities. Suppose further the availability of three lasers with frequencies ν_{10} , ν_{20} , and ν_{21} , that, respectively, can stimulate transitions between the first level and the ground state, the second level and the ground state, and the second level and the first level. For example, $h\nu_{20} = \epsilon_2 - \epsilon_0$, where h is Planck's constant. If one of these incoherent lasers illuminates the ensemble of atoms for a time long compared to the Rabi period, the populations in the corresponding pair of levels will be equalized. The maximum energy is extracted when the correct sequence of laser pulses is applied.

Now suppose that the accessible states have energies with numerical values $\vec{\epsilon} = (0, 1, 4)$ and the initial state densities are $\vec{n} = (0, 2/7, 5/7)$, where the sum has been normalized to 1. Then, the initial energy is $W_0 = 22/7$. The energy at step j can be written as W_j . The sequence of level-equalizing steps (ν_{21} , ν_{20} , and ν_{10}) then gives

$$\begin{array}{ll} \epsilon_0 = 0 & \epsilon_1 = 1 & \epsilon_2 = 4 \\ \text{initial} & W_0 = 22/7 & \begin{pmatrix} 0 & 2/7 & 5/7 \\ 0 & 1/2 & 1/2 \\ 1/4 & 1/2 & 1/4 \\ 3/8 & 3/8 & 1/4 \end{pmatrix} \\ \text{step 1} & W_1 = 5/2 & \\ \text{step 2} & W_2 = 3/2 & \\ \text{step 3} & W_3 = 11/8 & \end{array}$$

The energy extracted is thus $22/7 - 11/8 = 99/56$ or approximately 56% of the initial plasma energy. This work will demonstrate that the sequence of pulses used here is optimal and results in the minimum-energy final state, or equivalently the maximum possible extracted energy. What is of interest,

however, is how exactly this can be proved, how the maximum extraction can be calculated efficiently, and how the complexity of the problem increases with the number of states.

It turns out that the answer to these questions lies in the mathematical developments in other fields (although these developments appear not to have received much attention). Similar level-mixing operations have been considered in chemical reaction kinetics.⁷ More directly of use here, Zylka identified the set of accessible states through level-mixing operations, called the K set, using as an example the problem of attainable temperatures in heat reservoirs pairwise connected by heat pipes, with an arbitrary number of reservoirs.⁸ Thon and Wallace, in the context of characterizations of altruism as a pairwise relaxation correction to economic inequality,⁹ derived further features of the K set.¹⁰

Using these characterizations of the K set, the sequence of operations to extract maximal energy can be found. Although K , the set of states that can be reached from these level-mixing operations, is not convex,⁸ one can imagine covering the entirety of K with a small convex polygon. This polygon (namely, the *convex hull* of K , denoted $ch(K)$ here) is determined by taking all possible convex combinations of the points found within K . Equipped now with a linear objective function (the total energy of a state) and a convex feasible region (the unique covering polygon, $ch(K)$), we may apply the fundamental theorem of linear programming to locate the minimum energy state at a vertex or edge joining two or more vertices of the convex hull of K . Crucially, K contains each of the vertices of its convex hull (by construction), and so, the minimum energy state over the polygon *covering* K is identical to the minimum energy state found *within* K .

Thus, using the results of Zylka and of Thon and Wallace, for the three-level system, we shall pose and answer the following five questions:

- (1) What sequence minimizes the energy?
- (2) What is the full set of sequences that must be considered before the optimal sequence can be found?
- (3) What are the full set of sequences that could possibly be a solution, for some values of the energy levels and the initial population densities?
- (4) If it were possible to partially relax the distribution between two states, rather than fully relax it, would that ever be a useful step?
- (5) Is it the case that it is ever useful to take a step that increases the energy rather than decreases it?

The paper is organized as follows. In Sec. II, we define the diffusion model. In Sec. III, we reproduce results of the space of relaxation solutions and show how this immediately answers the first three questions. In Sec. IV, we answer the fourth question, proving that partial relaxation is never a useful step, regardless of the number of states. In Sec. V, we demonstrate out that strategies previously considered² can be put more precisely and further prove for any number of states that energy-increasing steps can never be part of the optimal sequence. In Sec. VI, we offer further discussion of the implications for N states and the degree of complexity of the problem. In Sec. VII, we summarize the main conclusions.

II. DIFFUSION MODEL

Suppose a set of level energies $\epsilon = (\epsilon_1, \epsilon_2, \dots, \epsilon_N)$ and a set of initial populations $n_0 = (n_0^1, n_0^2, \dots, n_0^N)$. Here, we understand the symbols ϵ and n_0 , without superscripts, to represent vectors; the initial level density of state i is represented as n_0^i . Consider a diffusion operation that equalizes the populations of a pair of levels (i, j) such that

$$(n_0^i, n_0^j) \rightarrow \left(\frac{n_0^i + n_0^j}{2}, \frac{n_0^i + n_0^j}{2} \right) \quad (1)$$

leaving all other level populations unchanged. We are interested here in the minimization of the system energy $W_d \doteq \epsilon \cdot n_f$ after repeated application of operations of this type on an initial state n_0 and reaching a state n_f .

The diffusion operation (1) can be represented by doubly stochastic matrices of the form $B_{ij} = \frac{1}{2}(I + Q_{ij})$, where I is the $N \times N$ identity matrix and Q_{ij} is the permutation matrix that exchanges the i th and j th level populations. Application of B_{ij} equalizes the i th and j th populations. For example, (1) could be styled $n_0 \rightarrow n_0 B_{ij}$.

The B_{ij} are symmetric, idempotent, and do not generally commute. (Two B_{ij} commute if neither of them operates on the same level.) They are a particular case of the T -transform: $T = (1 - \alpha)I + \alpha Q$, $\alpha \in [0, 1]$ and Q is a permutation of the identity matrix which exchanges only two rows.¹¹ Like all doubly stochastic matrices, T -transforms are measure-preserving: $\sum_{ab} T_{ab} n_b = \sum_b n_b = 1$. It is important to distinguish between the cases of $0 \leq \alpha \leq 1/2$ and $1/2 < \alpha \leq 1$; the latter case corresponds to moving density from a less-populated level to a more-populated level. For now, we will consider only $\alpha = 1/2$ transforms, i.e., the B_{ij} .

III. THE SET OF POINTS K

Zylka was the first to identify the set of accessible states through level-mixing operations: the K set.⁸ K is determined by the provided set of level populations, represented as a length- N vector n_0 , as well as the allowed diffusion operations. Without loss of generality, n_0 may be ordered increasing, as we assume throughout this work. As described previously, the diffusive B_{ij} operations equalize the populations of any pair of levels i and j . Each element contained in K is an N -tuple of level populations that can be reached by applying some sequence of the various B_{ij} to the initial state n_0 .

The linear function W_d assumes its extremal values on the boundary of $ch(K)$. The three-level system is conveniently depicted in $n_1 - n_2$ space. Due to normalization of the population vector, one coordinate is ignorable and a general state n may be written as $n = (n_1, n_2, 1 - n_1 - n_2)$; if the total density is say 1, the density of the third is simply $1 - n_1 - n_2$. Following Zylka, we will demonstrate that K is star-like.⁸

To see this, first let us consider the example considered earlier, and previously,² namely, the case of $N = 3$ case with initial data $n_0 = (0, 2/7, 5/7)$ and $\epsilon = (0, 1, 4)$.

One can generate the entire set K by applying arbitrarily long sequences of the transforms B_{ij} to the initial point n_0 . We denote the set of points generated by k arbitrary B_{ij} the

k th generation of K . The first six generations of K are plotted in Figure 1, overlaid with $ch(K)$. Except for the original point n_0 , the entirety of K lies along three distinct line segments joining pairs of extreme points, as depicted in Figure 2. This arrangement is obvious if one considers that every state must have $n_i = n_j$, for some i and j , if the last transform applied in the sequence arriving at that state is B_{ij} .

The six extreme points (excepting n_0) can then be paired according to their final B_{ij} . For example, the extreme points $n_0 B_{12} B_{13}$ and $n_0 B_{23} B_{13}$ are so paired, and the line joining them satisfies $n_1 = n_3 = 1 - n_1 - n_2$, or $n_2 = 1 - 2n_1$. It is now clear that K must be star-shaped with respect to $e = (1/3, 1/3, 1/3)$ because the three lines joining pairs of extreme points satisfy $n_1 = n_2 = 1 - n_1 - n_2$ there.⁸ Likewise, $ch(K)$ for a three-level system is defined by at most seven extreme points (see Appendix A). Each generation approaches e more closely, and no extreme points are generated after the third generation.

(Consider the effect of B_{ij} on a state $n = (n_1, n_2, 1 - n_1 - n_2)$. Then, the Euclidean distance s of n from e satisfies $s^2 = (n - e) \cdot (n - e)$. Comparing the distances of n and nB_{ij} from e , one finds $(n - e) \cdot (n - e) - (nB_{ij} - e) \cdot (nB_{ij} - e) = \frac{1}{2}(n_i - n_j)^2 \geq 0$. Thus, each B_{ij} brings a state closer to e .)

Note that the set K is non-convex,⁸ since not all of the points in $ch(K)$ can be reached by sequences of B_{ij} applied to n_0 . Per the fundamental theorem of linear programming, the minimum W_d over the convex feasible region $ch(K)$ is found either at a single extreme point of $ch(K)$ or along an edge of $ch(K)$ joining two or more extreme points of $ch(K)$. (In the latter case, the minimum W_d multiplicity is equal to the number of collinear extreme points.) However, the extreme points of $ch(K)$ are all contained in K . Thus, the linearity of the objective function $W_d = \epsilon \cdot n$ ensures that it has the same minimum over K and $ch(K)$.

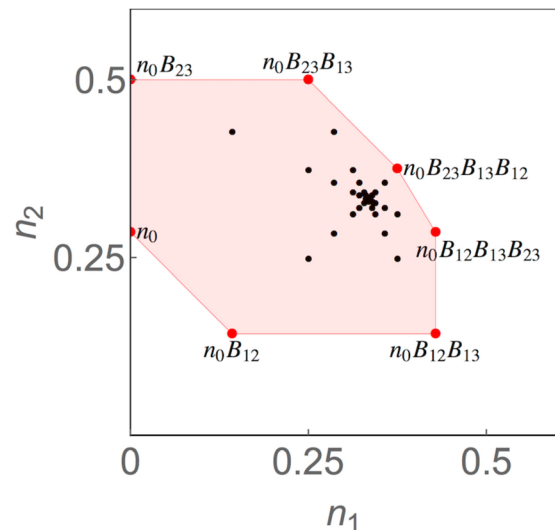


FIG. 1. The set K for $n_0 = (0, 2/7, 5/7)$, depicted in $n_1 - n_2$ space. The convex hull $ch(K)$ is illustrated by the pink region. Extreme points of $ch(K)$ are indicated with red dots and labeled by the series of transformations B_{ij} required to reach them. Interior points are labeled with small black dots. K itself is the union of the red and black dots.

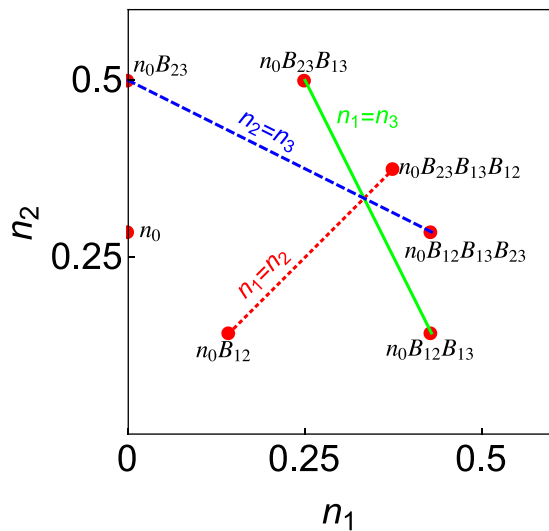


FIG. 2. The three lines covering K are depicted for $n_0 = (0, 2/7, 5/7)$, emphasizing the star-shaped nature of K .

Having identified the set of extreme points of $ch(K)$, $\mathcal{E}(ch(K))$, in Fig. 1, the minimum W_d may be computed as $\min\{\epsilon \cdot \mathcal{E}(ch(K))\}$. Fig. 3 overlays contours of the state energy $\epsilon \cdot n$ on K , thereby illustrating the scheme and identifying the minimum energy state. In this case, the optimum level populations are $n_f = n_0 B_{23} B_{13} B_{12} = (3/8, 3/8, 1/4)$, yielding a minimum $W_d = 11/8$, as previously calculated by exhaustive search.

The sequence which minimizes the plasma energy can always be identified with this algorithm. Crucially, because we have not assumed any ordering of the level energies ϵ , the slope of the state energy contours is arbitrary in the general case (cf. Fig. 3). Therefore, each of the seven extreme points identified is a possible solution to the energy minimization problem.

IV. PARTIAL RELAXATION

The discussion so far has assumed complete pairwise equalization of levels at every step, corresponding to B_{ij} transforms with $\alpha = 1/2$. From a physical standpoint, densities could also be relaxed through a diffusion process that only partially equalizes population levels, corresponding to the case of T -transforms with $0 < \alpha < 1/2$.

The $\alpha = 1/2$ transforms B_{ij} can be reached by repeatedly applying a particular T -transform with $0 < \alpha < 1$ formed from the same Q_{ij} , since for all $0 < \alpha < 1$, $\lim_{n \rightarrow \infty} T_{ij}^n = \frac{1}{2}(I + Q_{ij}) = B_{ij}$. Thus, the $\alpha = 1/2$ state space is in the closure of the state space for any fixed $0 < \alpha < 1$. At the same time, the $0 < \alpha < 1/2$ state space is contained entirely in the convex hull of the $\alpha = 1/2$ state space. To see this, simply observe that for $0 < \alpha < 1/2$,

$$T_{ij} = (1 - \alpha)I + \alpha Q_{ij} = (1 - 2\alpha)I + 2\alpha B_{ij}, \quad (2)$$

where $0 < 2\alpha < 1$. Thus, any $0 < \alpha < 1/2$ transform (on a state in the $\alpha = 1/2$ state space) results in a state that is a convex combination of the initial state and the state resulting from the corresponding $\alpha = 1/2$ transform, i.e., an interior point of

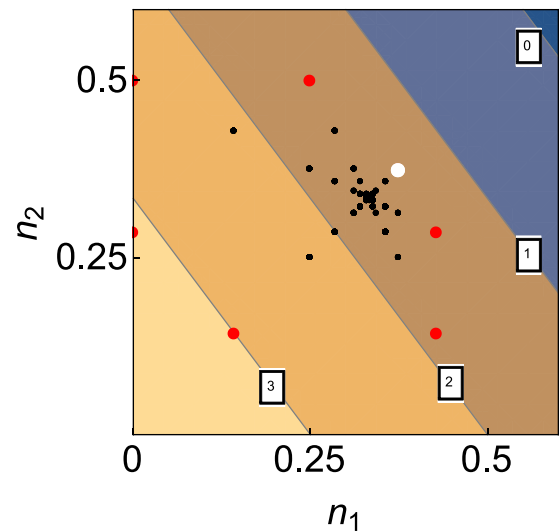


FIG. 3. K superimposed on contours of $W_d = \epsilon \cdot n$ (labeled by energy). The minimum W_d is found at the extreme point $n_0 B_{23} B_{13} B_{12} = (3/8, 3/8, 1/4)$ (labeled by a red circle in Figs. 1 and 2) labeled here by a large white circle.

$ch(K)$. See Fig. 4 for a depiction of these possibilities. For any T_{ij} with $0 < \alpha < 1/2$, the new state is constrained to lie on the dashed line joining p and the corresponding pB_{ij} .

It follows that it is sufficient to consider only $\alpha = 1/2$ transforms to identify the extreme points of the $0 < \alpha \leq 1/2$ state space and accordingly solve the energy minimization problem.

V. STRATEGIES FOR FINDING THE OPTIMUM SEQUENCE

Two strategies for determining the sequence of transforms B_{ij} required to attain the minimum- W_d state were conjectured in Ref. 2. Reproduced here, these strategies are:

- (1) Diffusion of particles first between similar population levels, all other things being equal, eventually releases more energy.

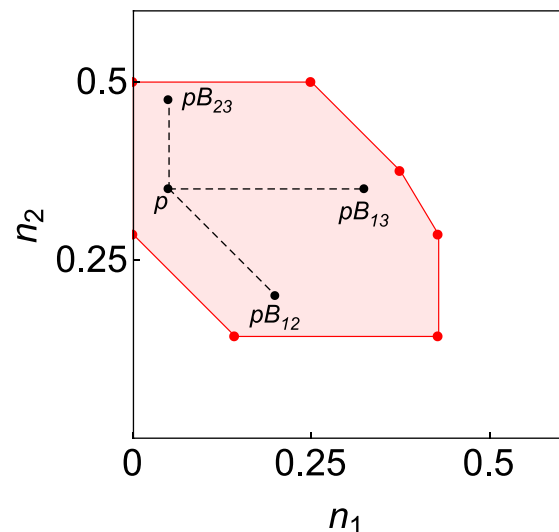


FIG. 4. Result of partial relaxations (T_{ij} with $0 < \alpha < 1/2$) applied to a point p in the convex hull of K for $n_0 = (0, 2/7, 5/7)$, as before. Partial relaxations result in interior points constrained to lie along the dashed lines joining p to each pB_{ij} .

- (2) Depleting of particles the higher energy level first, all other things being equal, eventually releases more energy.

These strategies were only surmised based on trial-and-error experience. However, it turns out that they are intimately related to the more precisely stated *Proposition 2*, proposed and proven by Thon and Wallace.¹⁰ It is worthwhile here to make use of the *permutation* of the set of initial populations, as introduced in Ref. 10. Given $n_0 = (n_1, n_2, n_3)$, the starting permutation is $\{1, 2, 3\}$ if $n_1 < n_2 < n_3$, as assumed throughout this work. Application of B_{ij} exchanges the level numberings, e.g., if n_0 has permutation $\{1, 2, 3\}$, $n_0 B_{12}$ has permutation $\{2, 1, 3\}$. For a more detailed exposition of these permutations and emergent combinatorial techniques, please refer to [Appendix B](#).

Put briefly, *Prop. 2* states that extreme points can be obtained by equalizing only *adjacent* level pairs. That is, any sequence of B_{ij} resulting in an extreme point will effect only adjacent transpositions in the population permutation. More concretely, $n_0 B_{12}$ and $n_0 B_{23}$ are both extreme points, but $n_0 B_{13}$, which averages the nonadjacent first and third levels, is not. However, $n_0 B_{12} B_{13}$ is an extreme point because the later application of B_{13} equalizes two adjacent levels, viz., $n_0 \sim \{1, 2, 3\} \rightarrow n_0 B_{12} \sim \{2, 1, 3\} \rightarrow n_0 B_{12} B_{13} \sim \{2, 3, 1\}$.

Because the initial populations are assumed ordered increasing and the global minimum energy state will always be located at an extreme point, any correct first step must be consistent with Strategy 1: the B_{ij} chosen must mix two adjacent levels.

It is clear that there are “dead ends” among the possible B_{ij} sequences, where a state is reached with level populations decreasing with level energy, such that no more energy can be extracted. Any such *stopping* state has the level population permutation, which is the reverse of the energy level permutation. For example, given $\epsilon = (\epsilon_1, \epsilon_2, \epsilon_3)$ with $\epsilon_2 < \epsilon_1 < \epsilon_3 \sim \{2, 1, 3\}$, the *stopping permutation* is $\{3, 1, 2\}$, such that $n_3 \leq n_1 \leq n_2$. $n \sim \{3, 1, 2\}$ can be reached from $n_0 \sim \{1, 2, 3\}$ by the sequence $n_0 B_{23} B_{13}$.

The three-level system has two extreme points with permutation $\{3, 2, 1\}$, the stopping permutation if the level densities and energies are both ordered increasing. In one case, the two lower-energy levels are first diffused; in the other, the two higher-energy levels are first diffused. The state energies of the extreme points cannot be ordered using a reduced set of variables (i.e., only some of the initial populations or energy levels), so the correct first step can only be determined in retrospect after a full calculation. The multiplicity of extreme points with a possible stopping permutation indicates that Strategy 2 is not generally applicable.

A further question of interest is the usefulness of an “annealing” strategy, whereby a diffusion operation heats the system, resulting in a state with extra energy. Subsequent B_{ij} would lower the system energy to its minimum value, presumably smaller than the minimum value possible without annealing. However, such a strategy cannot obtain a global minimum W_d . Note that any step which heats the system results in an inversion of the population permutation with respect to the correct stopping permutation. In order to obtain the stopping permutation, a subsequent diffusion operation is required on the two levels involved the heating step.

As an example, consider a case mentioned previously with level energy permutation $\epsilon \sim \{2, 1, 3\}$, initial population permutation $n_0 \sim \{1, 2, 3\}$, and stopping permutation $n \sim \{3, 1, 2\}$. Note that the initial permutation contains two inversions with respect to the stopping permutation. Applying B_{12} to the initial state results in the system absorbing energy

$$\epsilon \cdot n_0 B_{12} - \epsilon \cdot n_0 = \frac{1}{2}(n_2 - n_1)(\epsilon_1 - \epsilon_2). \quad (3)$$

By construction, each difference on the right hand side of Eq. (3) is positive and the system absorbs energy. Now consider the number of inversions: $n_0 B_{12}$ results in the level population permutation $n \sim \{2, 1, 3\}$, containing a total of three inversions with respect to the stopping permutation $\{3, 1, 2\}$. The extra inversion changes the parity of the permutation and requires at least one additional diffusion operation to correct. In particular, the same diffusion operation B_{12} must be repeated at some point in the relaxation process. *Prop. 3* of Ref. 10 states that a sequence of B_{ij} , which equalizes a particular pair of levels *more than once* cannot generate an extreme point of $ch(K)$. Even if all instances of the repeated B_{ij} correspond to adjacent transpositions, the necessary sequence will not yield an extreme point, which always has a (minimal length) reduced decomposition.

However, there exists at least one extreme point with the stopping permutation. Because K is star-shaped, any annealing strategy results in a non-optimal interior point (a convex combination of the uniform distribution e and an extreme point with the stopping permutation). Because the parity and number of inversions characterize any finite-length permutation, this conclusion holds in the general N -level case.

VI. COMPLEXITY

Given length- N initial data, there are at most $\binom{N}{2}$ possible states after one transformation has been applied (fewer in case of degeneracy in the initial level populations). The second generation contributes up to $N(N-1)(N-2)(N+5)/8$ unique states.¹² Although the number of possible unique states grows rapidly with the passing generations, these later states spiral quickly toward the uniform distribution $e = (1/N, 1/N, \dots, 1/N)$.

In fact, we can safely restrict our attention to the first $\binom{N}{2}$ generations, a nevertheless enormous set for large N . This follows from *Prop. 2*, which holds that extreme points are only generated from sequences of adjacent transpositions; the reverse permutation has the longest reduced decompositions, each containing $\binom{N}{2}$ adjacent transpositions. Therefore, every extreme point can be identified after only $\binom{N}{2}$ generations.

Thon and Wallace¹⁰ presented an algorithm for generating the extreme points of $ch(K)$. In fact, the algorithm identifies the reduced (minimum length) sequences of adjacent transpositions (i.e., permutations exchanging only neighboring elements in the set), leading to each permutation in the N th symmetric group S_N . For example, if $N=3$, the group S_3 contains $N!=6$

possible permutations. The permutation $\{3, 2, 1\}$ can be reached from the initial $X = \{1, 2, 3\}$ by two distinct sequences of adjacent transpositions: $(1, 2)(2, 3)(1, 2)$ and $(2, 3)(1, 2)(2, 3)$. The other five possible permutations of X have unique reduced decompositions in adjacent transpositions; the total number of such decompositions for all of the permutations in \mathcal{S}_3 is therefore seven.¹³ As noted, each possible permutation in \mathcal{S}_N is a stopping state for an appropriate permutation of ϵ .

Any sequence of diffusion operations with a repeated B_{ij} is not minimal and results in a permutation accessible with $\binom{N}{2}$ or fewer B_{ij} . This follows because the reverse permutation, the longest permutation when expressed in adjacent transpositions, requires precisely $\binom{N}{2}$ transpositions (corresponding to the number of inversions in the final permutation). For example, $nB_{23}B_{13}B_{12}B_{23}$ has the permutation $\{2, 3, 1\}$, which could also be reached with $nB_{12}B_{13}$.

In the $N = 3$ case, the minimization of W_d is straightforward. There are $\binom{3}{2} = 3$ unique B_{ij} : B_{12} , B_{13} , and B_{23} . Without loss of generality, the initial data n_0 are increasing, so the initial permutation is $\{1, 2, 3\}$. The set K is covered by $ch(K)$, which has seven extreme points: n_0 , n_0B_{12} , n_0B_{23} , $n_0B_{12}B_{13}$, $n_0B_{23}B_{13}$, $n_0B_{12}B_{13}B_{23}$, and $n_0B_{23}B_{13}B_{12}$.

There are ϵ for which each of the seven extreme points can serve as the optimum system configuration. As noted, $\epsilon \sim \{1, 2, 3\}$ is a special case in which the decomposition has maximum length $\binom{3}{2} = 3$; there are two unique decompositions of the stopping permutation $\{3, 2, 1\}$ in adjacent transpositions. Equivalently, there are two extreme points with the stopping permutation: the minimum system energy is then $W_d = \min\{\epsilon \cdot n_0B_{23}B_{13}B_{12}, \epsilon \cdot n_0B_{12}B_{13}B_{23}\}$. This is the most general scenario for the free energy optimization problem, in which multiple extreme points with the correct stopping permutation must be compared.

The problem has been reduced to evaluating the function $W_d = \epsilon \cdot n$ at a finite number of known extreme points. Unfortunately, the upper bound on the number of extreme points with stopping permutations is $\mathcal{O}(N^2)$.^{14,15} Because there is no *a priori* means of ordering these points in energy, the exponential depth of the state tree is intrinsic to the optimization problem.¹⁶ Thus, calculating the system energy accessible with discrete diffusive exchanges is NP-hard.

VII. CONCLUSIONS

By utilizing the (mostly ignored) literature on pairwise relaxation transformations, it is a relatively simple matter to apply the techniques of convex optimization and combinatorics to answer the questions posed. The first three questions posed have been resolved for a system with an arbitrary number of levels. The energy-minimizing sequence of B_{ij} is always located at an extreme point of $ch(K)$, and is in particular, a reduced decomposition of the stopping permutation. There may be as many as $\mathcal{O}(N^2)$ such decompositions for a given permutation, so many extreme points must be

considered before the optimal sequence can be found. However, each extreme point, i.e., each reduced decomposition in \mathcal{S}_N , is a possible solution for an appropriate set of energy levels and initial population densities. Moreover, partial relaxation or annealing strategies are never useful.

The exposition here has also laid the foundation for analyzing the extremal properties of more complicated systems. One might make use of the results about K to extremize nonlinear objective functions, as would be necessary in, e.g., systems with electrostatic self-energy. Alternately, formulating the optimization problem over a system of countable particles (as in integer programming) could shed light on the manipulation of degenerate matter. These systems and others like them could reveal the physical significance of the non-convexity of the state space.

Although we have shown that identifying the maximal energy extraction solution is impractical in most cases of interest, the results obtained along the way nonetheless provide useful constraints on diffusive schemes that should narrow the search for efficient strategies.

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APPENDIX A: EXTREME POINT GEOMETRY

Thon and Wallace proved¹⁰ that their algorithm generates the full set of extreme points for an arbitrary number of energy levels N . However, the $N = 3$ case admits a straightforward geometric proof. All states resulting from the application of a B_{ij} lie along the line $n_i = n_j$. This constrains the possible paths through state space. In particular, the slope of the line joining any two points p_1 and p_2 such that $p_2 = p_1B_{ij}$ is -1 if $(i, j) = (1, 2)$, 0 if $(i, j) = (1, 3)$, or ∞ if $(i, j) = (2, 3)$.

Fig. 5 plots the extreme points and the three lines covering K as well as these constrained trajectories. One extreme point is given (n , the initial data), and the other six are generated from choosing one of two routes through state space. Note that extreme points are only obtained by moving directly to a line $n_i = n_j$, without crossing any other such line. The lines are color-coded. Thus, for example, the partial relaxation along a red dotted line terminates on the red solid line; the red solid indicates complete relaxation of levels n_1 and n_2 , while all the states traversed along the dotted line are reachable. It can be seen from this geometrical representation that no extreme points are obtained by revisiting the same line: each diffusive transformation B_{ij} reduces the distance of the state from the uniform distribution e . Thus, a state that revisits a line would necessarily be interior to the first state reached on that line.

APPENDIX B: COMBINATORIAL METHODS

Thon and Wallace¹⁰ simplified the structures of many proofs by making use of the combinatorial features of the Dalton transfer problem.⁹ In particular, they introduced the permutation of the individuals whose incomes were to be redistributed. In their notation, the initial permutation is denoted $v = (v(1), v(2), \dots, v(N))$, where $v(i) = k$ is interpreted to mean that the individual numbered k is the i th poorest. This representation is equivalent to the common *two-line notation*

$$\begin{pmatrix} 1 & 2 & \cdots & N \\ v(1) & v(2) & \cdots & v(N) \end{pmatrix},$$

where the first row lists indices of the permutation and the second row identifies the individuals. Note that the ordering of the columns is immaterial. The first column could be read as “individual $v(1)$ is the poorest, listed first.” By analogy, the individuals of the Dalton problem may be construed as energy levels and likewise poor (rich) individuals are levels, which are smaller (larger) in population.

In our problem, it is assumed that the levels are ordered initially from least populated to most populated, yielding an initial permutation $v(i) = i$. Because the diffusion operations treated in this work transfer level densities but leave the level energies unchanged, we lose no generality by specializing to such a permutation, which we denote $\{1, 2, \dots, N\}$, reflecting $n_0^1 \leq n_0^2 \leq \dots \leq n_0^N$. (This is the *ordered arrangement* or *one-line* representation of the level density permutation.) In concordance with Ref. 10, we describe the levels nearest in population as *neighbors*, e.g., n_2 is neighbors with n_1 and n_3 only. It turns out that the extreme points of $ch(K)$ can be reached only by sequences of B_{ij} averaging such neighboring levels (Prop. 2 of Ref. 10).

Hoping for greater simplicity, we discuss separately the permutation of the level energies, denoted $\{w(1), w(2), \dots, w(N)\}$, with $w(i) = k$, meaning the level with the k th lowest energy has initially the i th smallest population. For example, if there is a complete population inversion, the highest-

energy levels are initially most populated and $\epsilon \sim \{1, 2, \dots, N\}$. If instead $N=3$ and the second-highest energy level is most populated, followed in turn by the lowest and highest energy levels, one has $\epsilon \sim \{3, 1, 2\}$, or, in two-line notation

$$\begin{pmatrix} 3 & 2 & 1 \\ 2 & 1 & 3 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix}.$$

(Recall our assumption $i = v(i)$, so that the first row of the two-line representation of the energy permutation identifies the states ordered by initial level populations. Thus the columns of the two-line representation could be parsed “greatest density in second-highest energy level, second-highest density in the lowest energy level, and least density in highest-energy level.”)

Apart from equalizing the populations of levels i and j , one can consider the effect of the B_{ij} on these permutations. As mentioned previously, the B_{ij} have no effect on the permutation of level energies, which remains fixed throughout the problem. However, each B_{ij} changes the permutation of level populations, with the result that the numberings are exchanged, so that, e.g., $n_0 B_{13}$ has permutation $\{3, 2, 1\}$. Considering the problem in $n_1 - n_2$ space, one realizes that the effect of a B_{ij} is to move the system state to another of the $N! = 6$ cells in $ch(K)$, each corresponding to a specific permutation of the level populations (cf. Fig. 1 of Ref. 10). The cells are separated by rays from e to six of extreme points in $ch(K)$ (n_0 excluded).

One of the key insights of this approach is the connection between population inversions and inversions in the permutation of level densities vis-à-vis the energy permutation. Using only the B_{ij} , it is possible to reorder the entire set of level populations, so that the final distribution is decreasing with energy (we term the permutations corresponding to such distributions *stopping* permutations).

In fact, there is a unique stopping permutation in a given problem: the *reverse* of the energy permutation, i.e., $\{w(N), w(N-1), \dots, w(1)\}$, obtained from the composition of \mathbf{w} with the order-reversing permutation. Let \mathbf{w}^r denote the reverse of the permutation \mathbf{w} . In two-line notation, one has

$$\begin{aligned} \mathbf{w}^r &= \begin{pmatrix} 1 & 2 & \cdots & N \\ w(1) & w(2) & \cdots & w(N) \end{pmatrix} \begin{pmatrix} 1 & 2 & \cdots & N \\ N & N-1 & \cdots & 1 \end{pmatrix} \\ &= \begin{pmatrix} N & N-1 & \cdots & 1 \\ w(N) & w(N-1) & \cdots & w(1) \end{pmatrix} \begin{pmatrix} 1 & 2 & \cdots & N \\ N & N-1 & \cdots & 1 \end{pmatrix} \\ &= \begin{pmatrix} 1 & 2 & \cdots & N \\ w(N) & w(N-1) & \cdots & w(1) \end{pmatrix}. \end{aligned}$$

Note that the reverse operation is an involution, such that $(\mathbf{w}^r)^r = \mathbf{w}$. For example, $\{1, 2, 3\}$ and $\{3, 2, 1\}$ are reverse permutations. In our previous example, the level energy permutation was $\{3, 1, 2\}$ such that $\epsilon_3 \leq \epsilon_1 \leq \epsilon_2$ for $\epsilon = (\epsilon_1, \epsilon_2, \epsilon_3)$ and $n_0 = (n_0^1, n_0^2, n_0^3)$. The reverse of the ϵ permutation is $\{2, 1, 3\}$. Thus, any stopping state has $n_2 \leq n_1 \leq n_3$, such that the final population in the highest-energy level (“level 2,” when ordered by initial population) is smallest, and so on.

By identifying the level energies’ permutation and its reverse, the search for the correct sequence of B_{ij} can be greatly narrowed because only extreme points with the stopping permutation need be considered.

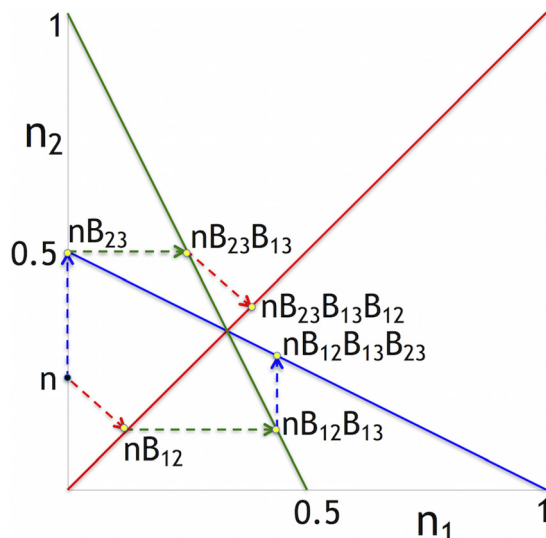


FIG. 5. Geometric construction of K . Extreme points of $ch(K)$ (yellow dots) depicted with lines $n_i = n_j$ (solid) and lines joining extreme points (dashed).

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