On the trail of the 2-body reduced density matrix ☆

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ABSTRACT

A brief review is made of developments in the theory of reduced density matrix estimation of fermion system properties, to which John Coleman contributed enormously. Emphasis is placed upon those constraints that are peculiar to the system in question, as well as to those of "universal" validity. The former are typically obtained by following the consequences of the insertion or deletion of one of the particles of the system, and, for example, the PY equation of classical fluid theory is identified as the "saturation" of a valid inequality. An analogous process for fermion systems is introduced but not carried out very far.

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John Coleman was a master of tight mathematical analysis. I first became aware of him in the early 1960's. A bunch of us had chatted extensively (at various Washington, DC meetings of the American Physical Society) about how to take advantage of Mayer's insightful—but deeply flawed—pair reduction of the *N*-fermion problem [1], and had nibbled away at its edges. Lowdin [2] had organized much of reduced density matrix technology without really advancing its basics. Then, Coleman dipped in, concisely formulated its essence [3], and raised the activity to what might be termed a professional level. The tight formulation gave the field the imprimateur of universality, and in later years, it was applied to quantum information theory as well [4]. Coleman returned to the topic on occasion [5], and in his later years, developed more interest in its applicability to specific physical problems [6]. He did not have the same confidence in the uncontrolled approximations endemic to this activity, and we were in contact on several occasions on such issues.

I would like to present an elaboration of a viewpoint I have emphasized of late [7], in which the explicit nature of the system of interest leads to enhanced control of fermion systems. I am sure that Coleman would have approved and would of course have made major contributions along these lines. Alas, this was not to be.

1. Introduction

Nature has provided theoretical physical scientists with a wonderful gift: the many orders of magnitude between the spatial structural scales of the basic constituents of matter and that of their electronic and nuclear components, which can then be characterized by a very small number of parameters—mass, charge, spin, etc. Coupled with the fantastic accuracy of basic dynamical laws, these might appear to reduce questions in the physical sciences to the "mere" working out of associated mathematics. Would that were the case (and it would then be pretty boring!). Of course, it all depends upon precisely what one means by mathematics.

Traditional mathematics is woefully inadequate in the treatment of many-body systems—those composed of many *identical indistinguishable* particles (no formal restriction since one can expand the space on which they live to incorporate defining characteristics—mass, spin, charge, ...). In our discussion, relating very much to work in progress, we want to emphasize *one philosophical and two technical points*.

The *philosophical* point is that, however we define the "solution" of the system, we are *not going to get exact solutions*, except perhaps for illustrative models, and in practice, exquisite detail would be obvious overkill, What we really want are results at a decent—perhaps cartoonish—level of resolution to produce an overall picture which however *we know how to sequentially improve*. **Inequalities** bounding the level of uncertainty, are clearly the tools of choice, unfamiliar though they may be.

The *first* technical point—or is it philosophical?—is that *few-body sums*, because the identity of the bodies is in principle unavailable, in fact sample the whole system, and are expected to be basic in any description. In particular, the powerful variational principles for few-body interacting systems will be expressed in such terms (and when they are not, as with entropy, their variation can be so expressed, and this will suffice). The problem here is to *guarantee that an N-body system* is the hidden generator.

The *second* technical point is that, when many particles are in question, collective "fluid" description is clearly called for, but one must make sure that the *fluid* is not infinitely divisible, i.e. is composed of *discrete particles*.

2. Prototype-ground state of classical lattice gas

Suppose the particles of a static *N*-body system interact only pairwise (in fact, all interactions can be developed from successive contact with an enveloping fluid of "quanta"), and are subject to an external field as well. For definiteness, the particles live on a lattice of Ω sites. Then the system (potential) energy takes the form

$$\Phi = \sum_1^N u(x_i) + \frac{1}{2}\sum_1^N{}' v(x_i, x_j)$$

where the prime $'$ signifies $i \neq j$, avoiding specific self-interaction terms. Now at what *microstate—the set of locations x_i—*is the lowest value of Φ achieved? For a conceptual simplification, introduce the single and pair site occupations

$$n(x) = \sum_1^N \delta(x, x_i)$$

$$n_2(x, y) = \sum_1^N{}' \delta(x, x_i)\delta(y, x_j) \qquad [= n(x)(n(y) - \delta(x, y))]$$

in which case

$$\Phi = \sum_x u(x)n(x) + \frac{1}{2}\sum_{x,y} v(x, y)n_2(x, y).$$

This relation is *linear* in the pair density, and of course in that of the strictly dependent

$$n(x) = 1/(N-1)\sum_y n_2(x, y).$$

For an *ensemble*, a *convex* linear combination of microstate densities, it then remains valid, with Φ, n, n_2 replaced by their ensemble averages:

$$\mathbf{\Phi} = \sum_x u(x)\mathbf{n}(x) + \frac{1}{2}\sum_{x,y} \mathbf{n}_2(x, y).$$

Minimization of $\mathbf{\Phi}$ over the ensemble of microstates is now guaranteed by convexity to produce the *same energy* and (if non-degenerate) the same microstate as the original microstate minimization.

This looks great! $\mathbf{n}$ and $\mathbf{n}_2$, while still non-negative and normalized, are not confined to integers, and we seem to have reduced our *N*-body minimization problem to a *proxy* 2-body problem. This need not be the case because we still must be sure that, e.g. $\mathbf{n}_2$ can be obtained as an average of **some** collection of microstates. Let us crawl before we walk.

(a) Suppose the lattice has only *2 sites*, A and B (see Fig. 1), and $N = 3$ particles are to be partitioned between these. The microstates are then (S, T) where $S + T = 3$, and S and T integers $\geqslant 0$. An ensemble results from weights $w(S, T)$ where $\sum w(S, T) = 1$ and $0 \leqslant w(S, T)$. It follows that $\mathbf{n}_2(A, A) = 3w(3, 0) + w(2, 1); \cdots$ $\mathbf{n}_2(B, B) = w(1, 2) + 3w(0, 3)$, or converting to relative frequencies $p = \mathbf{n}/6$ that

$$p_{AA} = \frac{1}{2}w(3, 0) + \frac{1}{6}w(2, 1) \ldots p_{BB} = \frac{1}{6}w(1, 2) + \frac{1}{2}w(0, 3)$$

and these are solvable for the $w(S, T)$ if and only if, S and T lie in the region shown: $1 \geqslant p_{AA} + p_{BB} \geqslant \frac{1}{3}, p_{AA}, p_{BB} \geqslant 0$.
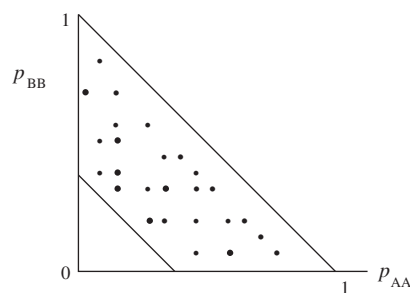

Fig. 1. Allowed space for three particles on two sites.

(b) $N \to \infty$ on a 2-site lattice. Now, $n_2(A, A) = S(S - 1), \ldots, n_2(B, B) = T(T - 1)$, so that $S = \frac{1}{2} + \sqrt{(n_2(A, A) + \frac{1}{4})}$, $T = \frac{1}{2} + \sqrt{(n_2(B, B) + \frac{1}{4})}$.

It follows that the microstates satisfy

$$N = 1 + \sqrt{\left(n_2(A, A) + \frac{1}{4}\right)} + \sqrt{\left(n_2(B, B) + \frac{1}{4}\right)}.$$

Now, with $p = n_2/N(N - 1)$ and $N \to \infty$, we obtain at once

$$\sqrt{p_{AA}} + \sqrt{p_{BB}} = 1,$$

whose convex extension, Fig. 2, is considerably more restrictive than in the previous few-particle case: the fluid limit imposes unphysical constraints.

(c) We proceed to a lattice of Ω sites, but rapidly go over to the fluid limit, in which $N \to \infty$, but uniformly. The microstates are again determined by the singlet site occupations $n(x)$, in terms of which the pair occupations are clearly

$$n_2(x, x) = n(x)(n(x) - 1)$$
$$n_2(x, y) = n(x)n(y) \text{ for } y \neq x.$$

We want to be able to enforce putative ensemble pair densities,

$$\mathbf{n}_2(x, y) = \sum_{\{x_i\}} w\{x_i\} \ n_2(x, y|\{x_i\}),$$

where $w\{x_i\} \geqslant 0$ and $\sum_{\{x_i\}} w\{x_i\} = 1$

by requiring a suitable set of inequalities

$$\sum_{x,y} C(\mu|x, y) \ \mathbf{n}_2(x, y) \geqslant 0$$

which are also sufficient. For the latter to hold, we specialize to microstates n_2. Doing so we have

$$\sum_{x,y} C(\mu|x, y)n(x)(n(y) - \delta(x, y)) \geqslant 0$$

for all matrices $C(x, y)$ in the set of inequalities.
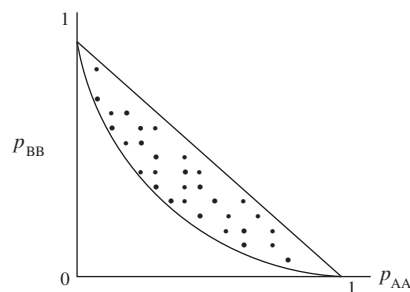Equivalently, if $N \to \infty$ uniformly, we set $p(x) = n(x)/N$ and obtain

Fig. 2. Allowed space for $N \to \infty$ particles on two sites.