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FINAL TECHNICAL REPORT

2/17/10

AFOSR GRANT FA9550-07-1-0084 BASIC STUDIES IN PLASMA PHYSICS 2/1/07–2/1/10

by

Joel L. Lebowitz

Department of Mathematics and Physics

Hill Center

Rutgers University

New Brunswick, NJ 08903

Principal Investigator

1. Space Charge Limited Flow in a Rectangular Geometry

We studied the spatial structure of the space charge limited current and electric field in a rectangle of arbitrary aspect ratio. The cathode and anode form two horizontal sides of the rectangle and a strong magnetic field forces the current to flow perpendicular to the electrodes. Using conformal mapping techniques we calculate the electric field outside this rectangle for any given potential distribution on its vertical boundaries. Inside the current rectangle we have a nonlinear Poisson equation with extra boundary conditions for two unknown functions: The potential and the current density. Both exhibit singular behavior at the edges of the rectangle. A semianalytic approximate method is developed for this unusual boundary value problem: We first match the boundary fields inside and outside the current region and then, using trial functions consistent with these matching conditions, we apply the least square technique and iterations to construct the solution in the current region. The analysis of the flow shows that the current wings are similar for all currents wider than one of the square cross noindent. There is also evidence that the total current does not vanish when the width goes to zero. The method of calculation appears generalizable to various geometries of vacuum and solid state devices.

2. Ionization in a 1-Dimensional Dipole Model

We study the evolution of a one dimensional model atom with δ -function binding potential, subjected to a dipole radiation field $E(t)x$ with $E(t)$ a $2\pi/\omega$ -periodic real-valued function. Starting with $\psi(x, t = 0)$ an initially localized state and $E(t)$ a trigonometric polynomial, complete ionization occurs; the probability of finding the electron in any fixed region goes to zero. For $\psi(x, 0)$ compactly supported and general periodic fields, we construct a resonance expansion. Each resonance is given explicitly as a Gamow vector, and is $2\pi/\omega$ periodic in time and behaves like the exponentially growing Green's function near $x = \pm\infty$. The remainder is given by an asymptotic power series in $t^{-1/2}$ with coefficients varying with x .

3. Erratum- Propagation Effects on the Breakdown of a Linear Amplifier Model: Complex-Mass Schrodinger Equation Driven by the Square of Gaussian Field

The proof of the inequality $\lambda_q(x, t) \leq (q\mu_{x,t} - 0^+)^{-1}$ [p 750, below Eq. (29)] is based on the statement that $\mathcal{E}(x, t; s)$ is an entire function of $s \in \mathbb{C}^M$ [see below Eq. (30)]. But according to Equation (9) and Lemma 1, all we know is that $\mathcal{E}(x, t; s)$ is an entire function of $k(s) \in \mathbb{R}^N$. Nevertheless, the above inequality holds, hence the proposition 1.

4. Entropy of Open Lattice Systems

We investigate the behavior of the Gibbs-Shannon entropy of the stationary nonequilibrium measure describing a one-dimensional lattice gas, of L sites, with symmetric exclusion dynamics and in contact with particle reservoirs at different densities. In the hydrodynamic scaling limit, L to infinity, the leading order ($O(L)$) behavior of this entropy has been shown by Bahadoran to be that of a product measure corresponding to strict local equilibrium; we compute the first correction, which is $O(1)$. The computation uses a formal expansion of the entropy in terms of truncated correlation functions; for this system the k -th such correlation is shown to be $O(L^{-k+1})$. This entropy correction depends only on the scaled truncated pair correlation, which describes the covariance of the density field. It coincides, in the large L limit, with the corresponding correction obtained from a Gaussian measure with the same covariance.

5. Percolation Phenomena in Low and High Density Systems

We consider the 2D quenched-disordered q -state Potts ferromagnets and show that at self-dual points any amalgamation of $q - 1$ species will fail to percolate despite an overall (high) density of $1 - q^{-1}$. Further, in the dilute bond version of these systems, if the system is just above threshold, then throughout the low temperature phase there is percolation of a single species despite a correspondingly small density. Finally, we demonstrate both phenomena in a single model by considering a “perturbation” of the dilute model that has a self-dual point. We also demonstrate that these phenomena occur, by a similar mechanism, in a simple coloring model invented by O. Häggström.

6. Space Charge Limited Two-dimensional Unmagnetized Flow in a Wedge Geometry

This paper studies the space charge limited current in an infinite wedge geometry in two dimensions. This geometry permits a reduction of the problem to a set of easily solved ordinary differential equations. The system, though very simplified, exhibits features similar to those expected to occur in many realistic systems with inhomogeneous electric fields. We obtain, in particular, a universal form for the particle trajectories and a non-monotone charge distribution with accumulation at both the cathode and the anode. The explicit solution of the model can be useful for testing numerical schemes. The case of a very low density current is also considered. Relaxation of the geometrical limitations of the model are studied using conformal mapping techniques. Possible applications to realistic systems, which can be tested by simple experiments, are presented.

7. Correlation Inequalities for Spin Glasses

We prove a correlation type inequality for spin systems with quenched symmetric random interactions. This gives monotonicity of the pressure with respect to the strength of the interaction for a class of spin glass models. Consequences include existence of the thermodynamic limit for the pressure and bounds on the surface pressure. We also describe other conjectured inequalities for such systems.

8. On a Random Matrix Models of Quantum Relaxation

In paper [7] two of us (J.L. and L.P.) considered a matrix model for a two-level system interacting with a $n \times n$ reservoir and assuming that the interaction is modelled by a random matrix. We presented there a formula for the reduced density matrix in the limit $n \rightarrow \infty$ as well as several its properties and asymptotic forms in various regimes. In this paper we give the proofs of assertions, announced in [7]. We present also a new fact about the model (see Theorem 2.1) as well as additional discussions of topics of [7]

9. Realizability of Point Processes

There are various situations in which it is natural to ask whether a given collection of k functions, $\rho_j(\mathbf{r}_1, \dots, \mathbf{r}_j)$, $j = 1, \dots, k$, defined on a set X , are the first k correlation functions of a point process on X . Here we describe some necessary and sufficient conditions on the ρ_j 's for this to be true. Our primary examples are $X = \mathbb{R}^d$, $X = \mathbb{Z}^d$, and X an arbitrary finite set. In particular, we extend a result by Ambartzumian and Sukiasian showing realizability at sufficiently small densities $\rho_1(\mathbf{r})$. Typically if any realizing process exists there will be many (even an uncountable number); in this case we prove, when X is a finite set, the existence of a realizing Gibbs measure with k body potentials which maximizes the entropy among all realizing measures. We also investigate in detail a simple example in which a uniform density ρ and translation invariant ρ_2 are specified on $\mathbb{Z}$; there is a gap between our best upper bound on possible values of ρ and the largest ρ for which realizability can be established.

10. From Time-symmetric Microscopic Dynamics to Time-Asymmetric Macroscopic Behavior: An Overview

Time-asymmetric behavior as embodied in the second law of thermodynamics is observed in *individual macroscopic* systems. It can be understood as arising naturally from time-symmetric microscopic laws when account is taken of a) the great disparity between microscopic and macroscopic scales, b) a low entropy state of the early universe, and c) the fact that what we observe is the behavior of systems coming from such an initial state—not all possible systems. The explanation of the origin of the second law based on these ingredients goes back to Maxwell, Thomson and particularly Boltzmann. Common alternate explanations, such as those based on the ergodic or mixing properties of probability distributions (ensembles) already present for chaotic dynamical systems having only a few degrees of freedom or on the impossibility of having a truly isolated system, are either unnecessary, misguided or misleading. Specific features of macroscopic evolution, such as the diffusion equation, do however depend on

the dynamical instability (deterministic chaos) of trajectories of isolated macroscopic systems. The extensions of these classical notions to the quantum world is in many ways fairly direct. It does however also bring in some new problems. These will be discussed but not resolved.

11. Displacement Convexity and Minimal Fronts at Phase Boundaries

We show that certain free energy functionals that are not convex with respect to the usual convex structure on their domain of definition, are strictly convex in the sense of displacement convexity under a natural change of variables. We use this to show that in certain cases, the only critical points of these functionals are minimizers. This approach based on displacement convexity permits us to treat multicomponent systems as well as single component systems. The developments produce new examples of displacement convex functionals, and, in the multicomponent setting, jointly displacement convex functionals.

12. Exact Results for Ionization of Model Atomic Systems

We present rigorous results for quantum systems with both bound and continuum states subjected to an arbitrary strength time-periodic field. We prove that the wave function takes the form of a sum of time-periodic resonant states with complex quasi-energies and dispersive part of the the solution given by a power series in $t^{-1/2}$. Generally, the imaginary part of each resonance is negative, leading to ionization of the atom, but we also give examples where the ionization rate is zero implying the existence of a time-periodic Floquet bound state. The complex quasi-energy has a convergent perturbation expansion for small field strengths.

13. Emergent Phenomena

Statistical mechanics relates the behavior of macroscopic objects to the dynamics of their constituent microscopic entities. Primary examples include the entropy increasing evolution of nonequilibrium systems and phase transitions in equilibrium systems. Many aspects of these phenomena can be captured in greatly simplified models of the microscopic world. They emerge as collective properties of large aggregates, i.e. macroscopic systems, which are independent of many details of the microscopic dynamics.

14. Vortices in the two-dimensional simple exclusion process.

We show that the fluctuations of the partial current in two dimensional diffusive systems are dominated by vortices leading to a different scaling from the one predicted by the hydrodynamic large deviation theory. This is supported by exact computations of the variance of partial current fluctuations for the symmetric simple exclusion process on general graphs. On a two-dimensional torus, our exact expressions are compared to the results of numerical simulations. They confirm the logarithmic dependence on the system size of the fluctuations of the partial flux. The impact of the vortices on the validity of the fluctuation relation for partial currents is also discussed.

15. Effect of Phonon-phonon Interaction on Localization

We study the heat current J in a classical one-dimensional disordered chain with on-site pinning and with ends connected to stochastic thermal reservoirs

at different temperatures. In the absence of anharmonicity all modes are localized and there is a gap in the spectrum. Consequently J decays exponentially with system size N . Using simulations we find that even a small amount of anharmonicity leads to a $J \propto 1/N$ dependence, implying diffusive transport of energy.

16. Striped Phases in Two-Dimensional Dipole Systems

We prove that a system of discrete two-dimensional 2D in-plane dipoles with four possible orientations, interacting via a three-dimensional 3D dipole-dipole interaction plus a nearest neighbor ferromagnetic term, has periodic striped ground states. As the strength of the ferromagnetic term is increased, the size of the stripes in the ground state increases, becoming infinite, i.e., giving a ferromagnetic ground state, when the ferromagnetic interaction exceeds a certain critical value. We also give a rigorous proof of the reorientation transition in the ground state of a 2D system of discrete dipoles with six possible orientations, interacting via a 3D dipole-dipole interaction plus a nearest neighbor antiferromagnetic term. As the strength of the antiferromagnetic term is increased, the ground state flips from being striped and in plane to being staggered and out of plane. An example of a rotator model with a sinusoidal ground state is also discussed.

17. Periodic Minimizers in 1D Local Mean Field Theory

Using reflection positivity techniques we prove the existence of minimizers for a class of mesoscopic free-energies representing 1D systems with competing interactions. All minimizers are either periodic, with zero average, or of constant sign. If the local term in the free energy satisfies a convexity condition, then all minimizers are either periodic or constant. Examples of both phenomena are given. This extends our previous work where such results were proved for the ground states of lattice systems with ferromagnetic nearest neighbor interactions and dipolar type antiferromagnetic long range interactions.

18. Time's Arrow and Boltzmann's Entropy

The arrow of time expresses the fact that in the world about us the past is distinctly different from the future. Milk spills but doesn't unspill; eggs splatter but do not unsplatter; waves break but do not unbreak; we always grow older, never younger. These processes all move in one direction in time - they are called "time-irreversible" and define the arrow of time. It is therefore very surprising that the relevant fundamental laws of nature make no such distinction between the past and the future. This in turn leads to a great puzzle - if the laws of nature permit all processes to be run backwards in time, why don't we observe them doing so? Why does a video of an egg splattering run backwards look ridiculous? Put another way: how can time-reversible motions of atoms and molecules, the microscopic components of material systems, give rise to the observed time-irreversible behavior of our everyday world? The resolution of this apparent paradox is due to Maxwell, Thomson and (particularly) Boltzmann. These ideas also explain most other arrows of time - in particular; why do we remember the past but not the future?

19. The Heat Conduction and Entropy Production in Anharmonic Crystals with Self Consistent Stochastic Reservoirs.

We investigate a class of anharmonic crystals in d dimensions, $d \geq 1$, coupled to both external and internal heat baths of the Ornstein-Uhlenbeck type. The external heat baths, applied at the boundaries in the 1-direction, are at specified, unequal, temperatures T_L and T_R . The temperatures of the internal baths are determined in a self-consistent way by the requirement that there be no net energy exchange with the system in the non-equilibrium stationary state (NESS). We prove the existence of such a stationary self-consistent profile of temperatures for a finite system and show it minimizes the entropy production to leading order in $(T_L - T_R)$. In the NESS the heat conductivity κ is defined as the heat flux per unit area divided by the length of the system and $(T_L - T_R)$. In the limit when the temperatures of the external reservoirs goes to the same temperature T , $\kappa(T)$ is given by the Green-Kubo formula, evaluated in an equilibrium system coupled to reservoirs all having the temperature T . This $\kappa(T)$ remains bounded as the size of the system goes to infinity. We also show that the corresponding infinite system Green-Kubo formula yields a finite result. Stronger results are obtained under the assumption that the self-consistent profile remains bounded.

20. Inheritance of Epigenetic Chromatin Silencing

Maintenance of alternative chromatin states through cell divisions pose some fundamental constraints on the dynamics of histone modifications. In this paper, we study the systems biology of epigenetic inheritance by defining and analyzing general classes of mathematical models. We discuss how the number of modification states involved plays an essential role in the stability of epigenetic states. In addition, DNA duplication and the consequent dilution of marked histones act as a large perturbation for a stable state of histone modifications. The requirement that this large perturbation falls into the basin of attraction of the original state sometimes leads to additional constraints on effective models. Two such models, inspired by two different biological systems, are compared in their fulfilling the requirements of multistability and of recovery after DNA duplication. We conclude that in the presence of multiple histone modifications that characterize alternative epigenetic stable states, these requirements are more easily fulfilled.

21. On the Two Species Asymmetric Exclusion Process with Semi-Permeable Boundaries.

We investigate the structure of the nonequilibrium stationary state (NESS) of a system of first and second class particles, as well as vacancies (holes), on L sites of a one-dimensional lattice in contact with first class particle reservoirs at the boundary sites; these particles can enter at site 1, when it is vacant, with rate α , and exit from site L with rate β . Second class particles can neither enter nor leave the system, so the boundaries are semi-permeable. The internal dynamics are described by the usual totally asymmetric exclusion process (TASEP) with second class particles. An exact solution of the NESS was found by Arita. Here we describe two consequences of the fact that the flux

of second class particles is zero. First, there exist (pinned and unpinned) fat shocks which determine the general structure of the phase diagram and of the local measures; the latter describe the microscopic structure of the system at different macroscopic points (in the limit L going to infinity in terms of superpositions of extremal measures of the infinite system. Second, the distribution of second class particles is given by an equilibrium ensemble in fixed volume, or equivalently but more simply by a pressure ensemble, in which the pair potential between neighboring particles grows logarithmically with distance. We also point out an unexpected feature in the microscopic structure of the NESS for finite L : if there are n second class particles in the system then the distribution of first class particles (respectively holes) on the first (respectively last) n sites is exchangeable.

22. Pattern Formation in Systems with Competing Interactions

There is a growing interest, inspired by advances in technology, in the low temperature physics of thin films. These quasi-2D systems show a wide range of ordering effects including formation of striped states, reorientation transitions, bubble formation in strong magnetic fields, etc. The origins of these phenomena are, in many cases, traced to competition between short ranged exchange ferromagnetic interactions, favoring a homogeneous ordered state, and the long ranged dipole-dipole interaction, which opposes such ordering on the scale of the whole sample. The present theoretical understanding of these phenomena is based on a combination of variational methods and a variety of approximations, e.g., mean-field and spin-wave theory. The comparison between the predictions of these approximate methods and the results of MonteCarlo simulations are often difficult because of the slow relaxation dynamics associated with the long-range nature of the dipole-dipole interactions. In this note we will review recent work where we prove existence of periodic structures in some lattice and continuum model systems with competing interactions. The continuum models have also been used to describe micromagnets, diblock polymers, etc.

23. Modulated phases of a one dimensional sharp interface model in a magnetic field

We investigate the ground states of 1D continuum models having short-range ferromagnetic type interactions and a wide class of competing longer-range antiferromagnetic type interactions. The model is defined in terms of an energy functional, which can be thought of as the Hamiltonian of a coarse-grained microscopic system or as a mesoscopic free energy functional describing various materials. We prove that the ground state is simple periodic whatever the prescribed total magnetization might be. Previous studies of this model of frustrated systems assumed this simple periodicity but, as in many examples in condensed matter physics, it is neither obvious nor always true that ground states do not have a more complicated, or even chaotic structure.

24. Heat conduction and phonon localization in disordered harmonic crystals

We investigate the steady state heat current in two and three dimensional disordered harmonic crystals in a slab geometry, connected at the boundaries to

stochastic white noise heat baths at different temperatures. The disorder causes short wavelength phonon modes to be localized so the heat current in this system is carried by the extended phonon modes which can be either diffusive or ballistic. Using ideas both from localization theory and from kinetic theory we estimate the contribution of various modes to the heat current and from this we obtain the asymptotic system size dependence of the current. These estimates are compared with results obtained from a numerical evaluation of an exact formula for the current, given in terms of a frequency transmission function, as well as from direct nonequilibrium simulations. These yield a strong dependence of the heat flux on boundary conditions. Our analytical arguments show that for realistic boundary conditions the conductivity is finite in three dimensions but we are not able to verify this numerically, except in the case where the system is subjected to an external pinning potential. This case is closely related to the problem of localization of electrons in a random potential and here we numerically verify that the pinned three dimensional system satisfies Fourier's law while the two dimensional system is a heat insulator. We also investigate the inverse participation ratio of different normal modes.

25. Droplet minimizers for the Gates-Lebowitz-Penrose free energy functional

We study the structure of the constrained minimizers of the Gates-Lebowitz-Penrose free-energy functional $\mathcal{F}_{\text{GLP}}(m)$, non-local functional of a density field $m(x)$, $x \in \mathcal{T}_L$, a d -dimensional torus of side length L . At low temperatures, $\mathcal{F}_{\text{GLP}}$ is not convex, and has two distinct global minimizers, corresponding to two equilibrium states. Here we constrain the average density $L^{-d} \int_{\mathcal{T}_L} m(x) dx$ to be a fixed value n between the densities in the two equilibrium states, but close to the low density equilibrium value. In this case, a "droplet" of the high density phase may or may not form in a background of the low density phase, depending on the values n and L . We determine the critical density for droplet formation, and the nature of the droplet, as a function of n and L . The relation between the free energy and the large deviations functional for a particle model with long-range Kac potentials, proven in some cases, and expected to be true in general, then provides information on the structure of typical microscopic configurations of the Gibbs measure when the range of the Kac potential is large enough.

26. Phase diagram of the ABC model on an interval

The three species asymmetric ABC model was initially defined on a ring by Evans, Kafri, Koduvely, and Mukamel, and the weakly asymmetric version was later studied by Clincy, Derrida, and Evans. Here the latter model is studied on a one-dimensional lattice of N sites with closed (zero flux) boundaries. In this geometry the local particle conserving dynamics satisfies detailed balance with respect to a canonical Gibbs measure with long range asymmetric pair interactions. This generalizes results for the ring case, where detailed balance holds, and in fact the steady state measure is known only for the case of equal densities of the different species: in the latter case the stationary states of the system on a ring and on an interval are the same. We prove that in the N to

infinity limit the scaled density profiles are given by (pieces of) the periodic trajectory of a particle moving in a quartic confining potential. We further prove uniqueness of the profiles, i.e., the existence of a single phase, in all regions of the parameter space (of average densities and temperature) except at low temperature with all densities equal; in this case a continuum of phases, differing by translation, coexist. The results for the equal density case apply also to the system on the ring, and there extend results of Clincy et al.

27. Nonequilibrium stationary solutions of thermostated Boltzmann equation in a field

We consider a system of particles subjected to a uniform external force E and undergoing random collisions with "virtual" fixed obstacles, as in the Drude model of conductivity. The system is maintained in a nonequilibrium stationary state by a Gaussian thermostat. In a suitable limit the system is described by a self consistent Boltzmann equation for the one particle distribution function f . We find that after a long time $f(v, t)$ approaches a stationary velocity distribution $f(v)$ which vanishes for large speeds, i.e. $f(v) = 0$ for $|v| > v_{\max}(E)$, with $v_{\max}(E) \sim 1/|E|$ as $|E| \rightarrow 0$. In that limit $f(v) \sim \exp(-c|v|^3)$ for fixed v , where c depends on mean free path of the particle. $f(v)$ is computed explicitly in one dimension.

28. Necessary and sufficient conditions for realizability of point processes

We give necessary and sufficient conditions for a pair of (generalized) functions $\rho_1(\mathbf{r}_1)$ and $\rho_2(\mathbf{r}_1, \mathbf{r}_2)$, $\mathbf{r}_i \in X$, to be the density and pair correlations of some point process in a topological space X , e.g., $(R)^d$, $(Z)^d$, or a subset of these. This is an infinite dimensional version of the classical "truncated moment" problem. Standard techniques apply in the case in which there can be only a finite number of points in any compact subset of X . Without this restriction we obtain, for compact X , strengthened conditions which are necessary and sufficient for the existence of a process satisfying a further requirement—the existence of a finite third order moment. We generalize the latter conditions in two distinct ways when X is not compact.

29. Rounding of first order transitions in low-dimensional quantum systems with quenched disorder

We prove that the addition of an arbitrarily small random perturbation of a suitable type to a quantum spin system rounds a first order phase transition in the conjugate order parameter in $d \leq 2$ dimensions, or in systems with continuous symmetry in $d \leq 4$. This establishes rigorously for quantum systems the existence of the Imry-Ma phenomenon, which for classical systems was proven by Aizenman and Wehr.

30. Correlation inequalities for quantum spin system with quenched centered disorder

It is shown that random quantum spin systems with centered disorder satisfy correlation inequalities previously proved (arXiv:cond-mat/0612371) in the classical case. Consequences include monotone approach of pressure and ground

state energy to the thermodynamic limit. Signs and bounds on the surface pressures for different boundary conditions are also derived for finite range potentials.

31. Normal typicality and von Neumann's quantum ergodic theorem

We discuss the content and significance of John von Neumann's quantum ergodic theorem (QET) of 1929, a strong result arising from the mere mathematical structure of quantum mechanics. The QET is a precise formulation of what we call normal typicality, i.e., the statement that, for typical large systems, every initial wave function ψ_0 from an energy shell is "normal": it evolves in such a way that $|\psi_t\rangle \langle \psi_t|$ is, for most t , macroscopically equivalent to the micro-canonical density matrix. The QET has been mostly forgotten after it was criticized as a dynamically vacuous statement in several papers in the 1950s. However, we point out that this criticism does not apply to the actual QET, a correct statement of which does not appear in these papers, but to a different (indeed weaker) statement. Furthermore, we formulate a stronger statement of normal typicality, based on the observation that the bound on the deviations from the average specified by von Neumann is unnecessarily coarse and a much tighter (and more relevant) bound actually follows from his proof.

32. Space-charge effects in field emission: One dimensional theory

The current associated with field emission is greatly dependent on the electric field at the emitting electrode. This field is a combination of the electric field in vacuum and the space charge created by the current. The latter becomes more important as the current density increases. Here, a study is performed using a modified classical 1D Child- Langmuir description that allows for exact solutions in order to characterize the contributions due to space charge. Methods to connect the 1D approach to an array of periodic 3D structures are considered.

33. On the approach to thermal equilibrium of macroscopic quantum systems

We consider an isolated, macroscopic quantum system. Let H be a micro-canonical "energy shell," i.e., a subspace of the system's Hilbert space spanned by the (finitely) many energy eigenstates with energies between E and $E + \delta E$. The thermal equilibrium macro-state at energy E corresponds to a subspace H_{eq} of H such that $\dim H_{eq}/\dim H$ is close to 1. We say that a system with state vector ψ in H is in thermal equilibrium if ψ is "close" to H_{eq} . We show that for "typical" Hamiltonians with given eigenvalues, all initial state vectors ψ_0 evolve in such a way that ψ_t is in thermal equilibrium for most times t . This result is closely related to von Neumann's quantum ergodic theorem of 1929.

List of Publications

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