

A Solvable Model for a System of Coulomb Particles in R^2 with Homotopically Nontrivial Phase Space.

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Summary. - In view of constructing classical statistical mechanical models with homotopically nontrivial phase space, leading to unambiguous quantization schemes by the path integral method, a solvable model is discussed, consisting of a gas of Coulomb particles in R^2 , which may be located between the Dyson's circular ensemble systems and the physical 2-dimensional Coulomb gas.

A thorough discussion of the quantization procedures raises, even in the simplest cases, disturbing features. In particular, the well-known fact that canonical transformations do not commute with quantization leads on the one hand to the nonuniqueness of the quantization methods and on the other casts an ambiguous light on the several attempts made so far to set up field theories into a « simple » canonical form. Assigning an operator in Hilbert space to every canonical variable cannot be done without having to face ordering ambiguities for those observables classically described by smooth functions on the phase space. In fact different ways of doing it lead to different algebraic structures, often characterized by entirely distinct mathematical features.

Unexpected ways of by-passing the above difficulties appear when the phase space is compact. The first interesting fact is that the topology of the phase space enters the picture.

If the phase space P has genus zero, the whole structure is displayed—indeed not surprisingly—by harmonic analysis over the homogeneous space $M = G/K$, where G is the covering group of some invariance group of P considered as a manifold, and K

is the isotropy subgroup of a fixed point of P . Thus Weyl's quantization procedure can be performed.

However, in the cases when the fundamental group of P is nontrivial things are much richer in new features, in that they depend on the homology classes of the phase space through the periods of all the holomorphic two-forms one can build on it. The quantum theory one gets in such a case bears strong similarities to the ordinary case, at least in the limit of large periods, with Gaussian sums playing the role of Gaussian integrals ⁽¹⁾.

The last observation opens an interesting set of new questions. A different way of performing quantization is by the path integral method: for a given pair of points in P , say p_1 and p_2 , the quantum-mechanical propagator between them is the sum over all paths from p_1 to p_2 of $\exp[(i/\hbar)S]$, where S is the action along the path. Such a functional sum is highly nontrivial when there are paths between the given endpoints which are not deformable into one another, *i.e.* belong to different homotopy classes ⁽²⁾.

Let P have universal covering space M , with covering projection $q: M \rightarrow P$ which is locally homeomorphic. Corresponding to the path from p_m to p_n , ($p_m, p_n \in P$) in P , one has a set of paths in M from some fixed $p_m^* \in q^{-1}(p_m)$ to all the $p_n^* \in q^{-1}(p_n)$, j running through the elements of the fundamental group of P . Thus in M one has indeed to form path integrals to each of the preimages of p_n (notice that q must be used also to bring the Lagrangian from P to M) and then sum over j with suitable weighting phase factors. The latter are arbitrary, and should be chosen in such a way that a nontrivial global identity transformation implies no more than an overall phase factor for the propagator.

On the other hand, for pure imaginary time quantum mechanics formally becomes Brownian diffusion, and the Green's functions reveal a profound connection with another fundamental object of the theory of stochastic processes: the partition function. One of the most interesting consequences of the extended work by SINAI ⁽³⁾ on classical one-dimensional models in statistical mechanics is the connection he was able to establish between these models and certain measure theoretic problems in the theory of dynamical systems. A special role in the study of a wide class of these dynamical systems—namely Anosov diffeomorphisms and flows on compact manifolds—is played by the generalized ζ -function defined by RUELLE ⁽⁴⁾ in the following way.

Considered M as a topological space, let $t: M \rightarrow M$ be a mapping and $F: M \rightarrow \mathbb{C}$ a complex-valued function on M . The ζ -function of Ruelle is given by

$$(1) \quad \zeta(z|\exp[F]) = \exp \left[\sum_{n=1}^{\infty} \frac{z^n}{n} \sum_{p_m \in \text{fix} t^n} \left[\exp \left[\sum_{j=0}^{n-1} F(t^j \circ p_m) \right] \right] \right].$$

Its physical meaning can be understood by noticing how in the special case when t is the shift operation on the configuration space of a one-dimensional lattice gas system with periodic boundary conditions and interaction energy F , then $\zeta(z/F)$ is just a generating function for the partition function,

$$(2) \quad \zeta(z|F) = \exp \left[\sum_{n=1}^{\infty} \frac{z^n}{n} Z_n \right].$$

⁽¹⁾ M. RASETTI: in *Selected Topics in Statistical Mechanics*, edited by N. N. BOGOLUBOV jr. and V. N. FEDYANIN (J.I.N.R. Publ., Dubna, 1981).

⁽²⁾ C. M. DE WITT: *Ann. Inst. Henri Poincaré*, **11**, 153 (1969); L. S. SCHULMAN: *J. Math. Phys. (N. Y.)*, **12**, 304 (1971).

⁽³⁾ YA. G. SINAI: *Teor. Mat. Fiz.*, **11**, 248 (1972); *Vestn. Mosk. Univ. Ser. Mat. Mekh.*, **29**, 152 (1974).

⁽⁴⁾ D. RUELLE: *Invent. Math.*, **34**, 231 (1976).

It appears quite evident from (1) and (2) how critically the ζ -function may depend on the topology of M . Thus it is of the utmost interest to succeed in producing classical-model systems whose phase space has a nontrivial covering.

Dealing with the statistical properties of random matrices, DYSON introduced the concept of circular ensemble⁽⁵⁾, $E_c^{(n)}$. The latter is defined in the space U_n of unitary matrices of modality 2^n and rank N (modality 2^n denotes: for $n = 0$ symmetric, for $n = 1$ unitary and for $n = 2$ self-dual quaternion matrices, respectively) by the characteristic requirements:

i) the ensemble is invariant under every automorphism A of the space U_n into itself realized by the matrix transformation

$$(3) \quad A: U \rightarrow S_n U T_n, \quad U \in U_n,$$

where S_n, T_n are unitary matrices (symplectic for $n = 2$), mutually transposed ($S_n = T_n^t$) in the cases $n = 0, 2$;

ii) the matrix elements $\{U_{r,s}; r \leq s; r, s = 1, \dots, N\}$ are statistically independent random variables.

These requirements can be written in the form of equations for the probability $dP = \mathcal{P}_N(U) dU$ that an element of U_n will belong to the neighbourhood dU of a given $U \in U_n$, where $\text{vol}(dU) = \prod_{1 \leq r \leq s \leq N} dU_{r,s}$.

DYSON found that in $E_c^{(n)}$ the probability density function of finding the eigenvalues $\{u_j = \exp[i\varphi_j]; j = 1, \dots, N\}$ of U within the range $\{\theta_j \leq \varphi_j \leq \theta_j + d\theta_j; j = 1, \dots, N\}$ is given by

$$(4) \quad \mathcal{P}_N(\{\theta_j; j = 1, \dots, N\}) = C_{N,\mu} \prod_{1 \leq r \leq s \leq N} |\exp[i\theta_r] - \exp[i\theta_s]|^\mu,$$

where $C_{N,\mu}$ is a normalization constant and μ is the modality. Upon setting,

$$(5) \quad \mathcal{P}_N = \frac{1}{Z_N} \exp[-\beta H]$$

the probability distribution \mathcal{P}_N then mimics a canonical ensemble in the customary sense of statistical mechanics, whose Hamiltonian H is that of a set of N point particles of charge k free to move on a circle of radius one (units are suitably chosen) in a two-dimensional universe, mutually repelling through a Coulomb interaction, provided $\beta = 2\mu\pi/k^2$ (and $Z_N(\beta) = C_{N,\beta k^2/2\pi}^{-1}$). The Hamiltonian H has the form

$$(6) \quad H = -\frac{k^2}{2\pi} \sum_{1 \leq r \leq s \leq N} \ln |\exp[i\theta_r] - \exp[i\theta_s]|.$$

Of course β can only formally be thought of as an inverse temperature, in that it assumes only the discrete values $\beta_n = 2^{n+1}\pi/k^2$; $n = 0, 1, 2$; in correspondence with the orthogonal, unitary and symplectic circular ensembles, respectively. The statistical properties induced by (5) are of course regular and analytic if β is continued to arbitrary real positive values, but exhibit an interesting singular behaviour when β is extended

(5) F. J. DYSON: *J. Math. Phys. (N. Y.)*, **3**, 140 (1962).

to real negative values (which allows describing the singular part of the free energy of a system of charges with alternating signs).

In the present note we discuss the preliminary results concerning a linear chain model of classical Coulomb charges in \mathbf{R}^2 , whose interaction mimics (6), but is endowed with a homotopically nontrivial covering configuration space. The model is meant to be a solvable approximation to the conventional Coulomb gas, closer to the latter than that realized by Dyson's Hamiltonian.

The basic idea is to write—as DYSON—a Hamiltonian describing a one-dimensional system, associated with a (piecewise linear) curve \mathcal{A} designed in such a way as to go through all the charges in the system but to recover eventually 2-dimensionality in the construction of the partition function by a functional integration over a set of loops $\{\mathcal{A}\}$ such as to cover the whole \mathbf{R}^2 . The second feature is that each charge is equipped with an additional degree of freedom (a continuous classical spinlike variable, ranging from -1 to $+1$), allowing us to describe the motion of the charges themselves along \mathcal{A} . The final step is that each curve \mathcal{A} is parametrized in terms of a set of lengths $\{L_r\}$, in such a way that all the possible two-body interactions (characteristic of the 2-dimensional Coulomb gas) are indeed taken into account in the partition function, even though the Hamiltonian describes only a part of them (n.n. along \mathcal{A}).

Indeed each curve \mathcal{A} endows the charges with an intrinsic lexicographic ordering, whereby the concept of n.n. along \mathcal{A} can be defined: the Hamiltonian is then designed so as to include only n.n. Coulomb interactions. Varying \mathcal{A} by changing the set of parameters $\{L_r\}$ induces different lexicographic orderings and, therefore, exhausts all possible two-particle couplings. Finally the parametrization reconducts the functional integration over the set of all closed curves, to a simple configurational integration over the parameters $\{L_r\}$.

The Coulomb gas is not reproduced to its full extent, in that some of the two-body interactions weight in the partition function with higher multiplicity than that corresponding to the physical Coulomb gas. However, in the thermodynamic limit the correct distribution is somewhat reapproached, as one can check by explicit enumeration of the configurations (6).

Notice also that the additional variability of the distances induced by the site-spin variables equips the space of loops with a non-Euclidean structure: the phase space—as required—is not simply connected.

In the sequel the model will be shown to exhibit a critical behaviour, ascribable to its instability with respect to the boundary configurations in the thermodynamic limit, as surmised by DOBRUSHIN (7) and LEBOWITZ and MARTIN-LÖF (8).

The model Hamiltonian has the form

$$(7) \quad \hat{H} = -\frac{k^2}{2\pi} \sum_{s=1}^{N-1} \ln \left[\frac{1}{\varrho} L_r (1 - |s_{r-1} s_r|) \right],$$

where L_r ; $r = 1, \dots, N-1$ denotes the maximum distance between the $(r-1)$ -th and the r -th spins, whereas s_r ; $r = 0, 1, \dots, N-1$ is a continuous spin variable ranging in the interval $-1 \leq s_r \leq +1$. To begin with, free boundary conditions are assumed. ϱ is a characteristic length, fixing the scale of distances.

(6) C. BUZANO, V. PENNA and M. RASETTI: in preparation.

(7) R. L. DOBRUSHIN: *Theory Prob. Its Appl. (USSR)*, **10**(2), 209 (1965).

(8) J. LEBOWITZ and M. LÖF: *Commun. Math. Phys.*, **25**, 276 (1972).

It is self-evident that as all the s_r and L_r are let to vary over the whole allowed ranges, \hat{H} assumes—with higher multiplicity—the same values assumed by H as $\theta_r, \theta_s; r < s; r, s = 1, \dots, N$ range from 0 to 2π .

Denoting by L the length of the curve A , we define first the reduced partition function $Z_{N-1}(s_0)$ with the spin s_0 on the boundary kept fixed,

$$(8) \quad Z_{N-1}(s_0) = \frac{1}{2} (2\varrho)^{-(N-2)} \int_0^L dL_1 \dots \int_0^L dL_{N-1} \delta \left(L - \sum_{r=1}^{N-1} L_r \right) \int_{-1}^1 ds_1 \dots \int_{-1}^1 ds_{N-1} \exp[-\beta \hat{H}].$$

Here the Dirac delta-function takes care of the volume of the chain, whereas the integration over the variables $\{s_r; r \neq 0\}$ induces the desired multiplicity of the possible relative distances between nearest-neighbour pairs of spins; $\beta = (k_B T)^{-1}$.

The form of \hat{H} as given in eq. (7) allows the factorization of the reduced partition function $Z_{N-1}(s_0)$,

$$(9) \quad Z_{N-1}(s_0) = \mathcal{Z}_{N-1}(s_0) \varrho^{-(N-1)(\nu+1)} \int_0^L dL_1 L_1^\nu \dots \int_0^L dL_{N-1} L_{N-1}^\nu \delta \left(L - \sum_{r=1}^{N-1} L_r \right),$$

where

$$(10) \quad \mathcal{Z}_{N-1}(s_0) = \int ds_1 \dots \int ds_{N-1} \prod_{r=1}^{N-1} (1 - s_{r-1} s_r)^\nu$$

and $\nu = \beta k^2 / 2\pi$ ranges now over the whole \mathbf{R} .

By a trivial change of variables $\{L_r = Lx_r; r = 1, \dots, N-2\}$, after performing in eq. (9) the integration over L_{N-1} explicitly, the $(N-1)$ -tuple integral in $Z_{N-1}(s_0)$ is reduced to a generalized Dirichlet's⁽⁹⁾ integral

$$(11) \quad I(N, \nu) = \int_{D_{N-2}} \dots \int dx_1 \dots dx_{N-2} \prod_{r=1}^{N-2} x_r^\nu \left(1 - \sum_{r=1}^{N-2} x_r \right)^\nu$$

over the domain $D_{N-2} = \left\{ x_r; r = 1, \dots, N-2 \mid x_r \geq 0, \sum_{r=1}^{N-1} x_r \leq 1 \right\}$, whereby we have

$$(12) \quad Z_{N-1}(s_0) = \left(\frac{L}{\varrho} \right)^{(N-1)(\nu+1)} I(N, \nu) \mathcal{Z}_{N-1}(s_0).$$

By its very definition (10) $\mathcal{Z}_{N-1}(s_0)$ is the solution of the recursion relation

$$(13) \quad \mathcal{Z}_{N-1}(s_0) = \int_0^1 dt (1 - s_0 t)^\nu \mathcal{Z}_{N-2}(t).$$

In the thermodynamic limit, $N \rightarrow \infty$, (13) turns into the integral equation (where

(9) P. G. LEJEUNE DIRICHLET: *Werke hrsg. auf Veranlassung der Königlich. Preussischen Akademie der Wissenschaften*, edited by L. KRÖNECKER (Chelsea Publ. Co., Bronx, N. Y., 1969), p. 375.

we set $\mathcal{Z}(x) = \lim_{N \rightarrow \infty} \mathcal{Z}_N(x)$,

$$(14) \quad \mathcal{Z}(s_0) = \int_0^1 dt (1 - s_0 t)^\nu \mathcal{Z}(t).$$

A thorough analysis of eq. (14) shows that a solution $\mathcal{Z}(s_0)$ exists, convergent over the entire domain $|s_0| \leq 1$, only for $\nu > -1$ and integer. In particular, as $\nu \rightarrow -1^+$, the principal part (P) of $\mathcal{Z}(s_0)$ is given by

$$(15) \quad P(\mathcal{Z}(s_0)) \sim \frac{\pi}{\gamma} |s_0|^{-\frac{1}{2}} (1 - |s_0|)^{-\frac{1}{2}} {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; |s_0|\right),$$

where γ is the Euler-Mascheroni constant. The hypergeometric function in (15) is in fact a complete elliptic integral of the first kind, namely $K(|s_0|^{\frac{1}{2}})$, which for $|s_0| \rightarrow 1^-$ behaves like a logarithmic function: $[\ln 4 - \ln(1 - |s_0|^{\frac{1}{2}})]$. Thus $\mathcal{Z}(s_0)$ develops an instability as $|s_0|$ is varied so as to get the extreme values zero and one.

On the other hand, in eq. (11) the integration can be performed in a formal way explicitly

$$(16) \quad I(N, \nu) = \frac{[I(1 + \nu)]^{N-1}}{\Gamma[(N-1)(1 + \nu)]},$$

showing that $I(N, \nu)$ is itself analytic over the whole complex-plane, except at ν negative integer. The asymptotic form of (16) for large N is

$$(17) \quad I(N, \nu) \sim \frac{1}{(2\pi)^{\frac{1}{2}}} N^{-N(1+\nu)} |1 + \nu|^{-N(1+\nu)} \exp[N(1 + \nu)] [I(1 + \nu)]^N.$$

In order to compute the free energy per site f , one has finally to compute the complete partition function \tilde{Z}_N . The latter is defined in the following way. First one imposes periodic boundary conditions on the spins; $s_N = s_0$. Then

$$(18) \quad \tilde{Z}_N = 2 \left(\frac{I}{Q}\right)^{(N-1)(\nu+1)-1} I(N, \nu) \int_0^1 \mathcal{Z}_{N-1}(s_0) ds_0.$$

The integral on the r.h.s. of (18) is now equal to the trace of the N -th iterate $K^{(N)}(s_0, s_0)$ of the integral kernel operator

$$(19) \quad k(s_0, t) = (1 - s_0 t)^\nu.$$

Denoting by $\lambda_0 \geq \lambda_1 \geq \lambda_2 \dots$ the eigenvalues of the associated Fredholm integral equation of the second kind (compare with (14))

$$(20) \quad S[\Phi](s_0) = \int_0^1 dt (1 - s_0 t)^\nu \Phi(t) = \lambda \Phi(s_0),$$

one can write

$$(21) \quad \int_0^1 \mathcal{Z}_{N-1}(s_0) ds_0 = \sum_{n=0}^{\infty} \lambda_n^N,$$

so that the dimensionless free energy per spin in the thermodynamic limit ($N \rightarrow \infty$, $L \rightarrow \infty$, $L/N = \nu$ finite and fixed)

$$(22) \quad \tilde{f} = \frac{2\pi}{k^2} f = - \lim_{\substack{N \rightarrow \infty \\ L \rightarrow \infty \\ \frac{L}{N} = \nu}} \frac{1}{N|\nu|} \ln \tilde{Z}_N,$$

reads

$$(23) \quad \tilde{f} = \frac{1+\nu}{|\nu|} \left\{ \ln|1+\nu| - 1 + \ln\left(\frac{\rho}{\nu}\right) \right\} - \frac{1}{|\nu|} \ln[I(1+\nu)] - \frac{1}{|\nu|} \ln \lambda_0.$$

Equation (23) requires for the reality of the term $\ln[I(1+\nu)]$ that ν is a real number either > -1 or bounded below by a negative odd integer and above by the successive negative even integer: $-2n-1 < \nu < -2n$; $n = 1, 2, 3, \dots$

Further analysis of the behaviour of f demands a thorough investigation of the behaviour of λ_0 as a function of ν in the above domain.

To begin with, we notice that the integral operator S defined by (20) is always bounded for $\nu > -1$. For ν negative it is Sobolev's and has the following properties, for $\Phi \in \mathcal{L}_p(\Omega)$ (where $\mathcal{L}_p(\Omega)$ denotes a Lebesgue measure space defined over the bounded domain $\Omega = [0, 1]$; *i.e.* a Banach space with respect to the norm $\|\Phi\|_{\mathcal{L}_p} = \left\{ \int_0^1 |\Phi|^p dx \right\}^{1/p}$):

i) if $|\nu| < (1 - 1/p)$, S is a bounded linear operator $\mathcal{L}_p(\Omega) \rightarrow C^{0,\alpha}(\Omega)$, where $\alpha = \min\{1, (1 - 1/p + \nu)\}$; $0 < \alpha \leq 1$ and $C^{0,\alpha}$ denotes the space of Hölder continuous functions (solutions of the Poisson equation);

ii) if $|\nu| > (1 - 1/p)$, S is a bounded linear operator $\mathcal{L}_p(\Omega) \rightarrow \mathcal{L}_r(\Omega)$ with $r < p/(1 - p(1 + \nu))$.

Moreover, the matrix realization of S in an orthogonal polynomial basis, in the indicated ranges of ν has all its elements of absolute value less than one, and all but those in the first column strictly negative.

A simple application of Perron-Frobenius theorem shows then that λ_0 is always positive and less than 1, whereas it is unique for $\nu > -1$, degenerate otherwise.

This implies for the model under consideration an extremely rich variety of the phase diagram which shows different features depending on whether $\nu \geq 0$. Such a diagram is regular for $\nu > 0$, at $\nu = 0$ it exhibits a (possibly infinite) discontinuity for \tilde{f} , while in the case of negative ν it may show a (possibly infinite) number of phases separated by polar singularities, in a way somewhat similar to the ANNNI model⁽¹⁰⁾.

⁽¹⁰⁾ J. VILLAIN and P. BAK: *J. Phys. (Paris)*, **42**, 657 (1981).