FUNDAMENTAL PHASE SPACE IDENTITIES FOR GAUGE FIELDS IN SUPERFLUIDS AND SOLIDS

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We specify the fundamental path integral identities in phase space which govern the thermal fluctuations of superflow and vortex lines in superfluids as well as of stresses and defects in solids. The key role is played by two mutually dual gauge field systems. The identities are extended to comprise the full fluctuating differential geometries of the gauge systems.

The fluctuation arena of quantum mechanics and quantum statistics is defined by what we shall call a *fundamental phase space identity*:

$$1 \equiv \int \mathrm{d}x' \, \langle x't' | xt \rangle \equiv \int \mathscr{D}x \int \frac{\mathscr{D}p}{2\pi} \exp\left(\mathrm{i} \int_t^{t'} \mathrm{d}t \, p\dot{x} \right)$$

$$\equiv \int \frac{\mathrm{d}p'}{2\pi} \langle p't' | pt \rangle \equiv \int \mathscr{D}x \int \frac{\mathscr{D}p}{2\pi} \exp\left(-\mathrm{i} \int_t^{t'} \mathrm{d}t \, \dot{p}x \right). \tag{1}$$

It is the path integral equivalent of Heisenberg's uncertainty relation $[\hat{p}, \hat{x}] = -\mathrm{i}$ in the operator language of quantum physics. There it specifies the Hilbert space in which the state vectors evolve. Arbitrary quantum systems are described by subtracting, from the exponent, an imaginary time integral of the total energy $\mathrm{i}\int \mathrm{d}t \, [K(p) + V(x)]$ so that it becomes i times the classical action. Then, by dropping in (1) the left-hand integral $\int \mathrm{d}x'$ or $\int \mathrm{d}p'/2\pi$, one obtains the quantum mechanical amplitudes in the x or p representations. By placing under the integral a δ-function, $\delta(x-x')$ or $2\pi\delta(p-p')$, thereby making the paths in the action periodic in $t'-t$ and by continuing $t'-t$ to imaginary $-\mathrm{i}/k_\mathrm{B}T$, one obtains the full quantum partition function of the system at temperature T. ($\hbar=1$, k_B are the Planck and Boltzmann constants.) The phase space identity (1) is therefore truly fundamental in quantum and statistical physics and fully deserves its name.

The purpose of this paper is to present similar identities also for the classical statistical mechanics of fluctuating superflow and vortex lines in superfluids and of stresses and defects (comprising dislocations and disclinations) in solids. They involve two mutually dual gauge field systems, one for the superflow or the stresses, and one for the vortex or the defects lines.

Let us begin with the simpler case of superfluids where the fundamental phase space identity reads

$$1 = \int_{-\infty}^{\infty} \mathscr{D}b_i \int_{-\infty}^{\infty} \mathscr{D}\gamma \int_{-\infty}^{\infty} \mathscr{D}\gamma_i^\mathrm{p} \, \Phi[\gamma_i^\mathrm{p}] \exp\left(\mathrm{i} \int \mathrm{d}^3x \, [b_i(\partial_i\gamma - \gamma_i^\mathrm{p})] \right). \tag{2a}$$

Here γ is the phase variable of the superfluid condensate, b_i is the canonically conjugate superfluid current, and γ_i^p is what we may call (in analogy with the defect nomenclature below) the *plastic deformation* of the

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phase distortion [1,2] [#1]. It carries the information on the ensemble of vortex lines. It is a gauge field called *vortex gauge field.* The associated gauge transformations move Volterra sheets through space at fixed boundaries (which are the vortex lines) and read

$$\gamma_i^{\mathrm{p}} \to \gamma_i^{\mathrm{p}} + \partial_i N . \tag{3a}$$

They can be absorbed by a shift in the phase variable

$$\gamma \to \gamma + N . \tag{3b}$$

The functional $\Phi[\gamma_i^{\mathrm{p}}]$ serves to fix a convenient gauge, for instance $\gamma_3^{\mathrm{p}} = 0$ (axial gauge). Integrating out the γ fluctuations leads to the conservation law of superflow

$$\partial_i b_i \equiv 0 , \tag{4a}$$

which suggests introducing a *gauge field of superflow*, a_i, via

$$b_i = \epsilon_{ijk} \partial_j a_k , \tag{4b}$$

with b_i being invariant under the *superflow gauge transformation*

$$a_i \to a_i + \partial_i \Lambda . \tag{4c}$$

We therefore can go over to a double gauge field version of the identity (2a)

$$1 \equiv \int \mathscr{D} a_k \, \Psi[a_k] \int \mathscr{D} \gamma_i^{\mathrm{p}} \, \Phi[\gamma_i^{\mathrm{p}}] \exp\left(-\mathrm{i} \int \mathrm{d}^3 x \, b_i \gamma_i^{\mathrm{p}} \right) , \tag{2b}$$

where $\Psi[a_k]$ is a gauge fixing functional of a_k. A partial integration brings (2b) to the form

$$1 = \int \mathscr{D} a_k \, \psi[a_k] \int \mathscr{D} \gamma_i^{\mathrm{p}} \, \Phi[\gamma_i^{\mathrm{p}}] \exp\left(-\mathrm{i} \int \mathrm{d} x^3 \, a_i l_i \right) , \tag{2c}$$

where

$$l_i = \epsilon_{ijk} \partial_i \gamma^{\mathrm{p}} \tag{5a}$$

is the gauge invariant curl of the vortex gauge field. It satisfies the *vortex conservation*

$$\partial_i l_i = 0 \tag{4b}$$

and describes the *vortex density* of the superfluid. One can go one step further and rewrite (2c) in complete duality to (2a) as

$$1 \equiv \int \mathscr{D} a_k \, \Psi[a_k] \int \mathscr{D} l_i \int \mathscr{D} \theta \exp\left(\mathrm{i} \int \mathrm{d}^3 x \, (a_i - \partial_i \theta) l_i \right) , \tag{2d}$$

where the auxiliary θ integration enforces the vortex conservation law (4b). The full partition function of the superfluid with vortex lines is obtained by subtracting in the exponent $1/k_{\mathrm{B}}T$ times the energy of superflow, the leading term being

$$\beta E_{\mathrm{s}} = \tfrac{1}{2} \int \mathrm{d}^3 x \, b_i^2 . \tag{5a}$$

In the double gauge version (2b), we might also subtract an extra core energy of vortex lines

$$\beta E_{\mathrm{v}} = -\tfrac{1}{2} \tilde{\beta} \int \mathrm{d}^3 x_i \, l_i^2 . \tag{5b}$$

[#1] For a detailed presentation and further references see ref. [2].

If the field system is placed on a lattice and the vortex gauge field $\gamma_i^{\rm p}$ takes only discrete values ($\equiv$integer multiple of 2π) the resulting partition function becomes the well-known Villain model of the superfluid phase transition, which is known [2,3] to describe correctly the entire critical regime of superfluid ^{4}He [3].

We now turn to solids. If the molecules are small and there is little rotational stiffness, the fundamental phase space identity reads

$$1\equiv\int\mathscr{D}\sigma_{ij}\int\mathscr{D}u_i\int\mathscr{D}u_{ij}^{\rm p}\,\Phi[u_{ij}^{\rm p}]\,\exp\left(\mathrm{i}\int\mathrm{d}^3x\,\sigma_{ij}(\partial_iu_j+\partial_ju_i-2u_{ij}^{\rm p})\right), \tag{6a}$$

where σ_{ij} are the stress and u_i the dislacement fields, and $u_{ij}^{\rm p}$ is the plastic strain field. It is a *defect gauge field* with the *defect gauge transformations*

$$u_{ij}^{\rm p}\to u_{ij}^{\rm p}+\partial_iN_j+\partial_jN_i,\quad u_i\to u_i+N\,. \tag{7a}$$

Integrating out u_i shows that stress is conserved,

$$\partial_i\sigma_{ij}=0\,, \tag{8a}$$

so that there exists a stress gauge field χ_{ij} with [#2]

$$\sigma_{ij}=\epsilon_{ikl}\epsilon_{jmn}\partial_k\partial_m\chi_{ln} \tag{8b}$$

invariant under

$$\chi_{ln}\to\chi_{ln}+\partial_l\Lambda_n+\partial_n\Lambda_l\,. \tag{8c}$$

This permits rewriting (6a) in the double gauge form [3]

$$1\equiv\int\mathscr{D}\chi_{ij}\,\Psi[\chi_{ij}]\int\mathscr{D}u_{ij}^{\rm p}\,\Phi[u_{ij}^{\rm p}]\,\exp\left(-\mathrm{i}\int\mathrm{d}^3x\,\sigma_{ij}u_{ij}^{\rm p}\right). \tag{6b}$$

A partial integration gives

$$1\equiv\int\mathrm{d}\chi_{ij}\,\Psi[\chi_{ij}]\int\mathscr{D}u_{ij}^{\rm p}\,\Phi[u_{ij}^{\rm p}]\,\exp\left(-\mathrm{i}\int\mathrm{d}^3x\,\chi_{ij}\eta_{ij}\right), \tag{6c}$$

where

$$\eta_{ij}\equiv\epsilon_{ikl}\epsilon_{jmn}\partial_k\partial_mu_{ln}^{\rm p} \tag{7a}$$

is the defect gauge invariant *defect density* [4]. It satisfies the *defect conservation law*

$$\partial_i\eta_{ij}=0\,. \tag{7b}$$

If we subtract in the exponent the leading stress energy

$$\beta E_{\rm s}=-\frac{\mu^{-1}}{k_{\rm B}T}\int\mathrm{d}^3x\left(\sigma_{ij}^2-\frac{\nu}{1+\nu}\sigma_{ii}^2\right), \tag{8}$$

where μ is the shear modulus and ν the Poisson ratio, the partition function describes ensembles of defects and their proper long-range interactions in the continuum approximation. If desired, we may also introduce extra core energies for the defects by terms quadratic in η in analogy with (5b) for vortices. By placing the partition function on a lattice, and letting $n_{ij}^{\rm p}$ be integer multiples of the lattice spacing, we obtain the simplest model of defect mediated melting [5].

[#2] For a review of the use of the stress gauge field and its its history see ref. [4].

If the molecules in the solid are large, there is rotational stiffness and we have to extend the field variables by the angular degree of freedom $\omega_k=\frac{1}{2}\epsilon_{ijk}(\partial_i u_j-\partial_j u_i)$ and its canonical conjugate τ_{ij}, the torque stress [6]. The fundamental identity reads

$$1\equiv\int\mathscr{D}\sigma_{ij}\int\mathscr{D}\tau_{ij}\int\mathscr{D}u_i\int\mathscr{D}\omega_{ij}\int\mathscr{D}\beta^{\rm p}_{ij}\int\mathscr{D}\phi^{\rm p}_{ij}\,\Phi[\beta^{\rm p}_{ij},\phi^{\rm p}_{ij}]$$

$$\times\exp\left(\mathrm{i}\int \mathrm{d}^3x\,[\sigma_{ij}(\partial_i u_j-\epsilon_{ijk}\omega_k-\beta^{\rm p}_{ij})+\mathrm{i}\tau_{ij}(\partial_i\omega_j-\phi^{\rm p}_{ij})]\right), \tag{9}$$

where $\beta^{\rm p}_{ij}$ and $\phi^{\rm p}_{ij}$ are the plastic gauge fields of dislocations and disclinations. The *defect gauge transformations* are

$$\beta^{\rm p}_{ij}\to\beta^{\rm p}_{ij}+\partial_i N_j-\epsilon_{ijk}M_k,\quad \phi^{\rm p}_{ij}\to\phi^{\rm p}_{ij}+\partial_i M_j,\quad u_i\to u_i+N_i,\quad \omega_k\to\omega_k+M_k\,. \tag{10a}$$

Integrating over u_i and ω_i gives the *stress conservation law*

$$\partial_i\sigma_{ij}=0,\quad \partial_i\tau_{ij}=-\epsilon_{jkl}\sigma_{kl}\,. \tag{10b}$$

They are solved in terms of the *stress gauge fields* A_{lj}, h_{lj},

$$\sigma_{ij}=\epsilon_{jkl}\partial_k A_{lj},\quad \tau_{ij}=\epsilon_{ikl}\partial_k\delta_{lj}+b_{ij}A_{ll}-A_{ji}\,, \tag{11a}$$

with the *stress gauge transformations*

$$h_{lj}\to h_{lj}+\partial_l\xi_j-\epsilon_{ljk}\Lambda_k,\quad A_{lj}\to A_{lj}+\partial_l\Lambda_j\,. \tag{11b}$$

Using the stress gauge fields, the fundamental identity (9a) takes the double gauge form

$$1\equiv\int\mathscr{D}h_{lj}\int\mathscr{D}A_{lj}\,\Psi[h_{lj},A_{lj}]\int\mathscr{D}\beta^{\rm p}_{ij}\int\mathscr{D}\phi^{\rm p}_{ij}\,\Phi[\beta^{\rm p}_{ij},\phi^{\rm p}_{ij}]\exp\left(\mathrm{i}\int\mathrm{d}^3x\,(\sigma_{ij}\beta^{\rm p}_{ij}+\tau_{ij}\phi^{\rm p}_{ij})\right). \tag{9b}$$

A partial integration leads to the alternative exponent

$$\mathrm{i}\int\mathrm{d}^3x\,(A_{lj}\alpha_{lj}+h_{lj}\theta_{lj})\,, \tag{9c}$$

where

$$\alpha_{lj}=\epsilon_{lki}\partial_k\beta^{\rm p}_{ij}+\delta_{lj}\phi^{\rm p}_{kk}-\phi^{\rm p}_{jl},\quad \theta_{lj}\equiv\epsilon_{lki}\partial_k\phi^{\rm p}_{ij} \tag{12a}$$

are the defect gauge invariant *dislocation and disclination densities* with the defect conservation laws

$$\partial_l\alpha_{lj}=-\epsilon_{jkl}\theta_{kl},\quad \partial_l\theta_{lj}=0\,. \tag{12b}$$

By subtracting in the exponent a stress energy (8) plus terms quadratic in τ_{ij}, we obtain the partition function of dislocations and disclinations with their proper long-range interactions [7]. If desired we may also subtract extra core energies quadratic in the defect densities. After being put on a lattice, with discretized plastic gauge fields, this partition function has recently explained the two step melting process in two dimensions at larger angular stiffness [8].

The fundamental identities can be generalized to a non-linear differential geometric description of dislocations and disclinations [4]. In the neighbourhood of each point in a solid, with an arbitrary parametrization x^i, we introduce locally orthonormal non-holonomic coordinates [9] $\mathrm{d}x^\alpha\equiv\mathrm{d}x^i h^\alpha{}_i$ so that the metric is $g_{ij}=h^\alpha{}_i h_{\alpha j}$ (with the indices α, β being contracted via $\eta_{\alpha\beta}=\delta_{\alpha\beta}$). They serve as a local reference frame without dislocations. The dreibein fields $h^\alpha{}_i$ convert tensor indices from i to α and back. The covariant derivative of a tensor $t_{i\alpha}$ is $D_j t_{i\alpha}=\partial_j t_{i\alpha}-\Gamma_{ji}{}^k t_{k\alpha}-A_{j\alpha}{}^\beta t_{i\beta}$ where $\Gamma_{ij}{}^k$, $A_{j\alpha}{}^\beta$ are the ordinary and the spin connection. The curvature tensor is the covariant curl of Γ or A, e.g. $R_{ij\alpha}{}^{\beta}=h_{\alpha}{}^{k}h^{\beta}{}_{l}R_{ijk}{}^{l}=(\partial_i A_j-\partial_j A_i-[A_i, A_j])_{\alpha}{}^{\beta}$. The torsion of the space is $S_{ij}{}^{k}=\frac{1}{2}(\Gamma_{ij}{}^{k}-\Gamma_{ji}{}^{k})=-\frac{1}{2}h_{\alpha}{}^{k}\ ({}^{A}D_i h^{\alpha}{}_j-{}^{A}D_j h^{\alpha}{}_i)$ where ${}^{A}D_i h^{\alpha}{}_j\equiv D_i h^{\alpha}{}_j+A_{i\beta}{}^{\alpha}h^{\beta}_j$. The geometry allows for local translations under which

$$\delta_E x^{\alpha}\equiv x^{\alpha}+\xi^{\alpha},\quad \delta_E h^{\alpha}{}_i=D_i\xi^{\alpha}-(A_{\beta i}{}^{\gamma}-2S_{\beta i}{}^{\gamma})\xi^{\beta}\,, \tag{13a}$$

while $A_{i\alpha}{}^{\beta}$ transforms like an ordinary tensor

$$\delta_E t_{i\alpha}=\xi_i\partial_j t_{i\alpha}+(\partial_i\xi^k)t_{k\alpha}\,. \tag{13b}$$

In addition, there are local rotations with antisymmetric $\omega_{\alpha\beta}$,

$$\delta_L A_{i\alpha}{}^{\beta}=D_i\omega_{\alpha}{}^{\beta},\quad \delta_L h_{i\alpha}=\omega_{\alpha}{}^{\beta}h_{i\beta}\,. \tag{14b}$$

The fields $h_{\alpha i}$ and $A_{i\alpha}{}^{\beta}$ carry the information on the defects. They are the generalizations of the plastic gauge fields $\beta^{\rm p}_{ij}$, $\phi^{\rm p}_{i\alpha}{}^{\beta}\equiv\phi^{\rm p}_{ij}\epsilon_{j\alpha}{}^{\beta}/2$ of eq. (9).

Let us contract the curvature tensor and form the Einstein tensor $G_{ij}=R_{ij}-\frac{1}{2}g_{ij}R_k{}^k$ as well as the Palatini tensor $S_{ij,k}\equiv 2(S_{ijk}+g_{ik}S_{jl}{}^{l}-g_{jk}S_{il}{}^{l})$. They are the generalizations of dislocation and disclination densities $\alpha_{kij}\equiv\alpha_{kl}\epsilon_{lij}/2$, θ_{ij}:

$$\alpha_{kij}\equiv S_{ij,k},\quad \theta_{i\alpha}\equiv G_{\alpha i}\,. \tag{15}$$

They coincide with the canonical energy momentum tensor and the spin density of the gravitational field in general relativity [9]. The Bianchi identities, which in general relativity ensure energy momentum and angular momentum conservation of the gravitational field [2,9], guarantee now the *conservation of defects* as follows (generalizing (12b)):

$$D^*_i\theta_{\alpha}{}^{i}=-2S_{i\alpha}{}^{\gamma}\theta_{\gamma}{}^{i}-\tfrac{1}{2}A^{i\beta}{}_{\gamma}R_{\alpha i\beta}{}^{\gamma},\quad D^*_i\alpha^{i}{}_{\alpha}{}^{\beta}=\theta_{\alpha}{}^{\beta}-\theta^{\beta}{}_{\alpha}\,, \tag{16}$$

where $D^*_i=D_i-2S_{ij}{}^{j}$. Let us choose a specific local set of $\mathrm{d}x^{\alpha}$ coordinates, say $\mathrm{d}\bar{x}^{\alpha}$, by fixing the defect gauge (for instance $h^{\alpha}{}_3=\delta^{\alpha}{}_3$, $A_{3\alpha}{}^{\beta}=0$). The distorted crystal configurations may be parametrized by a total displacement field $u^{\alpha}(x^i)$. Then the fundamental phase space identity of a solid with dislocations and disclination reads

$$1\equiv\int\mathscr{D}\sigma_{\alpha}{}^{i}\int\mathscr{D}\tau^{i\alpha}{}_{\beta}\int\mathscr{D}u^{\alpha}\int\mathscr{D}\omega_{\alpha}{}^{\beta}\int\mathscr{D}h^{\alpha}{}_i\int\mathscr{D}A_{i\alpha}{}^{\beta}\,\Phi[h^{\alpha}{}_i, A_{i\alpha}{}^{\beta}]$$

$$\times\exp\!\left(\mathrm{i}\int\mathrm{d}^3x\,\sqrt{g}\,[\sigma_{\alpha}{}^{i}(D_i u^{\alpha}-\omega_i{}^{\alpha}-(A_{\beta i}{}^{\alpha}-2S_{\beta i}{}^{\alpha})u^{\beta}-h^{\alpha}{}_i)+\tau^{i\alpha}{}_{\beta}(D_i\omega_{\alpha}{}^{\beta}-A_{i\alpha}{}^{\beta})]\right), \tag{17}$$

where the conjugate variables $\sigma_{\alpha}{}^{i}$ and $\tau^{i\alpha}{}_{\beta}$ are again stresses and torque stresses, as in (9a) (which is obviously a linearized version of (17a)). Integrating out u^{α} and $\omega_{\alpha}{}^{\beta}$ gives the *stress conservation laws* (generalizing (10b))

$$D^*_i\sigma_{\alpha}{}^{i}=-2S_{\alpha i}{}^{\gamma}\sigma_{\gamma}{}^{i}-\tfrac{1}{2}\tau^{i\beta}{}_{\gamma}R_{\alpha i\beta}{}^{\gamma},\quad D^*\tau^{i\alpha}{}_{\beta}=\sigma^{\alpha}{}_{\beta}-\sigma_{\beta}{}^{\alpha}\,, \tag{18}$$

which have the same form as (16) for the defect densities. Notice that the stress gauge transformations (13a), (14a) are absorbed by the corresponding transformations of the displacement field

$$\delta_E u^{\alpha}=\xi^{\alpha},\quad \delta_L u^{\alpha}=\omega^{\alpha}{}_{\beta}u^{\beta}\,, \tag{19}$$

making (17a) *defect gauge invariant*. The crystal forces are now introduced by subtracting, in the exponent, an elastic energy, such as [6–8]

$$E_{\rm el}\equiv\tfrac{1}{4}\mu^{-1}\int\mathrm{d}^3x\,\sqrt{g}\left({}^{\rm s}\sigma_i{}^{j2}-\frac{\nu}{1+\nu}\,{}^{\rm s}\sigma_i{}^{i2}\right)+\tfrac{1}{8}(\mu l^2)^{-1}\int\mathrm{d}^3x\,\sqrt{g}\,\tau_{i\alpha}{}^{\beta}\tau^{i}{}_{\beta}{}^{\alpha}\,, \tag{20}$$

where ${}^{\rm s}\sigma_i{}^{j}$ is the symmetrized part of $h^{\alpha}{}_i\sigma_{\alpha}{}^{j}$. We can also add a similar term quadratic in the defect densities

$\alpha_{i\alpha\beta}$ and $\theta_{i\alpha}$ to account for extra core energies. In this way, we obtain a complete non-linear gauge field description of defects with their correct long-range forces.

As before, it is possible to express the stresses in terms of stress gauge fields which obviously play the same role for the stresses as $h_{\alpha i}$, $A_{i\alpha}{}^{\beta}$ do for the defect densities. This leads to the non-linear extension of the double gauge theory (9b). Moreover, due to the identical form of defect and stress conservation laws (16) and (18), one may want to consider the gauge theory of stresses as defining the differential geometry of the space, with the defects being the extra matter fields. The interpretation of the stress metric in this geometry is, however, not clear, so we shall refrain from presenting an explicit construction.

The fundamental phase space identities presented in this paper make it possible to study arbitrary ensembles of fluctuating superfluids and solids with the associated defects. It should be kept in mind, however, that a proper description of the most interesting aspects, the phase transitions, requires the generalization of the differential geometry to a discrete difference geometry, as in the lattice models studied in refs. [5] and [7].

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