# Charge-spin separation in 2D Fermi systems: Singular interactions as modified commutators, and solution of the 2D Hubbard model in the bosonized approximation

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The general two-dimensional fermion system with repulsive interactions (typified by the Hubbard model) is bosonized, taking into account the finite on-shell forward-scattering phase shift derived in earlier papers. By taking this phase shift into account in the bosonic commutation relations, a consistent picture emerges showing the charge-spin separation and anomalous exponents of the Luttinger liquid.

The proper description of the effect of finite forward-scattering on-shell phase shifts on Fermi systems for $D > 1$ (Ref. 1) has been the subject of a number of papers.[2-4] The existence of such scattering, leading to on-shell singularities in the $T$ matrix, was confirmed by Fukuyama and Narikiyo,[5] Metzner and di Castro,[6] and others. The discovery which these papers confirmed followed from the fact that when two particles are embedded in their respective Fermi seas, effectively all soft recoils are forbidden to them by the exclusion principle. Under these conditions, the logarithm of the $S$ matrix for relative motion retains a finite eigenvalue $\eta_0$ in two dimensions (2D),

$$S_0(Q) = \exp i[\eta_0(Q)] \; ,$$

in the limit that the relative momentum $Q = k_\uparrow - k'_\downarrow \to 0$, and that both states are below the Fermi level. (On general grounds, it seems likely that this can happen in 3D as well, but this has not been proven.) It is important to be clear that $S$ is not the conventional $T$ matrix defined for a hole at $k$ scattering against another at $k'$, whose imaginary part represents an incoherent decay process, vanishing at the Fermi surface; $S$ is the on-shell scattering matrix of particles embedded in the Fermi sea, and its phase determines the boundary condition for their asymptotic wave functions at the origin of relative coordinates $r - r' = 0$. Addition of a particle modifies the wave functions of all other particles, and our endeavor is to investigate the consequences of this fact.

Our initial description[7] was heuristic, merely pointing out that the effect of such a phase shift mimics that of a change in statistics by enforcing a partial exclusion principle between electrons of opposite spins. We also described the type of singular interaction which would give energy shifts similar to those which take place, and emphasized that these would "trash" Fermi-liquid theory. Some papers have focused on this singular interaction (specifically Engelbrecht and Randeria[2] and Stamp[3]). The treatment in terms of an interaction is in several respects unsatisfactory, as clarified by Baskaran.[4] But even Baskaran's discussion does not give us a clear insight into clean formal ways to deal with the situation.

The problem is that the effect is best thought of as a constraint on the wave functions, not as an interaction.

This is most clearly seen in the Hubbard model, where the effect of a strong enough repulsive potential $U \to \infty$ is to enforce a projective constraint, expressed as the Gutzwiller projector acting on the kinetic energy in the t-J model, for instance. Since the exchange term also is expressible purely in terms of projected operators, the t-J system is confined to the subspace defined by projected operators.

It is worth emphasizing that renormalization-group derivations of Fermi-liquid theory (FLT) as a theory of the low-energy states, such as that of Shankar, implicitly assume a free Fermion starting Hamiltonian. If the starting problem itself is projected onto a subspace, this property will remain after renormalization and FLT changes into the theory we shall derive.

In general (in 2D) the constraint appears as a phase shift, which is a boundary condition for the asymptotic wave function in the relative coordinates of a pair of particles. Such a wave function is indeterminate unless it has a boundary condition both at $|r - r'| \to \infty$ and at $r - r' \to 0$. Arguments in several of the original papers show that the rest of the particles may be satisfactorily dealt with by taking the exclusion principle into account; the multiparticle encounters are not crucial.

This local boundary condition on the asymptotic wave function at $r - r' \to 0$ is a kinematic, rather than a dynamic, effect: there is a change in the wave functions of the particles, not directly in their energy. We are used to this with hard-core potentials: the effect is best expressed as one purely on the kinetic energy, not on the potential. This kinematic effect dominates here because the scattering region where the potential acts is small, of order $N^{-1}$ compared to the asymptotic region in which the kinetic energy is modified. The way to make this point is that such a boundary condition can actually change the dimensionality of the Hilbert space of allowed wave functions. In simple terms, such a boundary condition forces the wave function's nodes to shift in such a way that a particle moves into or out of the distant boundary, so that the same volume contains $N \pm \eta/\pi$ particle states rather than $N$. This is what is meant by a change in the dimensionality of Hilbert space. This change of Hilbert space occurs in 1D even as a consequence of an ordinary interaction potential (hence the flexibility of statistics in 1D), but in all other dimensions it is distinct from the

       

kind of interaction effects which can be treated perturbatively.

The conclusion we came to is therefore that the effect of a finite phase shift is best modeled as a modification of the algebra of the particles, expressed in their commutation relations. Projected fermions

$$(c_{i\sigma}^+)_{\text{proj}} = P_G^i c_{i\sigma}^+ = (1 - n_{i-\sigma})c_{i\sigma}^+ \tag{1}$$

do not have the same commutation relations as ordinary fermions, obviously, but we have not found the fermion representation convenient to work with. It is much simpler to use the bosonized representation in terms of the Fermi-surface fluctuations.[8,9] The bosonized version of Fermi-liquid theory can be equivalently thought of as the appropriate gauge theory in the presence of a Fermi surface, since the bosonic variable is essentially the phase of the Fermi-surface wave function.

Haldane, particularly, has emphasized that the most useful description of the dynamics of a Fermi system is via the operators $\Delta k_F$ describing the position of the Fermi surface in $k$ space, taken to be dynamical variables, functions of a coarse-grained space, and time. That is, he argues that Luttinger's theorem holds exactly during sufficiently long-wavelength and low-frequency fluctuations. (Parenthetically, even the conventional derivations of Luttinger's theorem[10] depend not on the convergence of perturbation theory but merely on the assumption that excitations precisely at the Fermi surface (FS) do not decay; hence the Green's function is real.) We define operators

$$\Delta k_{F\sigma}(\Omega, r, t) \ ,$$

giving the Fermi-surface fluctuations of spin $\sigma$ at a point on the FS parameterized by $\Omega$, and at coarse-grained $r, t$. These are the bosonic variables: they commute for different $\Omega$ and $r$, and, for noninteracting electrons, for different $\sigma$. We can introduce a phase variable $\theta_\sigma$ of the wave function at the Fermi surface, which is a function of $\Omega$, $r$, and $t$, and then $\Delta k_{F\sigma}$ is

$$\Delta k_{F\sigma} = \hat{n}_\Omega \cdot \nabla \theta_\sigma \ , \tag{2}$$

where $\hat{n}_\Omega$ is the local normal to the fiduciary Fermi surface. $\theta$ and $\Delta k_F$, which is equivalent to the particle density at $\Omega, \rho(\Omega)$, are conjugate variables, and for free fermions have canonical commutation relations:

$$[\theta, \rho] = i\pi\delta(r - r')\delta(\hat{\Omega} - \hat{\Omega}') \ . \tag{3}$$

As Haldane has pointed out, this representation can be motivated by the idea of expressing the fermion field in terms of two real operators $\rho$ and $\theta$:

$$\psi(x) = \rho e^{i\theta(x)} \tag{4}$$

rather than by the earlier "Tomonaga" definition of $\rho(q)$ as a density of fermions $\sum_k c_{k+q}^+ c_k$. This latter representation is not possible when the fermions are projected operators. But we can still speak of a Fermi surface and a Fermi-surface phase for each spin which satisfies Luttinger's theorem, and hence determines the density of particles at each point on the Fermi surface. In this tran-

scription of the original idea of bosonization we follow Khveshchenko.[11] If a Fermi surface exists, this implies zero-frequency modes at each point on it, hence separate, independent conservation of particle and spin currents at the Fermi surface at each $\Omega$, even allowing for Fermi-surface fluctuations which may be integrably singular at low frequencies.

However, this does not imply that, in the presence of interactions, $\theta_\sigma$ and $\rho_\sigma$ (or $\Delta k_{F\sigma}$) remain the appropriate canonically conjugate variables. These are variables which measure, respectively, the particle number at a particular patch on the Fermi surface and a given spin and the phase of the wave function at the Fermi surface. If there is a finite phase shift for forward scattering of opposite-spin electrons, as we have shown,[1,7] the order of doing these operations matters. If we add a particle of up-spin, the phase of the down-spin wave function depends on whether the particle of up-spin was added before or after the phase was measured. The failure of commutation for opposite spins is the phase shift $\eta/\pi$, just as adding a particle of up-spin below the Fermi surface enforces a change in up-spin phase by the amount $\pi$. We may express this by writing the free-particle commutator in matrix form:

$$[\rho_\sigma, \theta_{\sigma'}]_{\text{bare}} = i\pi \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \delta(r - r')\delta(\Omega - \Omega') \ ,$$

$$\tag{5}$$

while

$$[\rho_\sigma, \theta_\sigma]_{\text{interacting}}$$

$$= i\pi \begin{bmatrix} 1 & \dfrac{\eta}{\pi} \\ \dfrac{\eta}{\pi} & 1 \end{bmatrix} \times \delta(r - r')\delta(\Omega - \Omega') \ . \tag{6}$$

Let us explain these equations in detail. Equation (5) means in the one-dimensional model that if we insert an extra particle into the Fermi sea at a point $r$, because of the exclusion principle the wave function at the Fermi surface [which is the basic interpretation of Eq. (4)] must have an extra node inserted into it near $r$; hence the phase difference between left- and right-going (or ingoing and outgoing) waves must shift by $\pi$ as a consequence. Hence after we insert one particle in $\rho$, $\theta$ will change by $\pi$, but not vice versa: one is the generator of displacements of the other. Equation (6) must be interpreted in exactly the same way. The insertion of an up-spin particle at $r$, near $\Omega$, means that the phase of the down-spin wave at $\Omega$ is shifted by $\eta$, while the up-spin wave is shifted by $\pi$. This means that $\theta_\uparrow, \rho_\uparrow$ and $\theta_\downarrow, \rho_\downarrow$ are no longer canonically conjugate; the correct canonically conjugate variables are proportional to

$$\theta_s = \frac{\theta_\uparrow - \theta_\downarrow}{\sqrt{2}} \ , \quad \rho_s = \frac{\rho_\uparrow - \rho_\downarrow}{\sqrt{2}} \tag{7}$$

and

$$\theta_c = \frac{\theta_\uparrow + \theta_\downarrow}{\sqrt{2}} \ , \quad \rho_c = \frac{\rho_\uparrow + \rho_\downarrow}{\sqrt{2}} \ . \tag{8}$$

The equations of motion of the charge and spin bosons follow from the commutation relations and the Hamiltonian, which as we explained is simply the original kinetic energy, the interaction terms being completely subsumed in the commutation relations. The Hamiltonian is, as for free particles, the one given by Haldane:

$$\mathcal{H} = \tfrac{1}{2} \int d\Omega \int d^D r \, v_F(\Omega) [\Delta k_F(\Omega), r, t)]^2$$

$$= \tfrac{1}{2} \int d\Omega \sum_q v_F [\rho^2(q, \Omega) + q^2 \theta^2(q, \Omega)] \; . \tag{9}$$

Then

$$[H, \theta_{c,s}(q, \Omega)] = v_{c,s} q \theta_{c,s}(q, \Omega) \; , \tag{10}$$

with

$$v_s = v_F(\Omega) \left[ 1 - \frac{\eta(\Omega)}{\pi} \right] \; ,$$

$$v_c = v_F(\Omega) \left[ 1 + \frac{\eta(\Omega)}{\pi} \right] \; , \tag{11}$$

and bosons are left as harmonic-oscillator variables with frequencies

$$\begin{bmatrix} q v_c & (\Omega) \\ q v_s & (\Omega) \end{bmatrix} \; .$$

For free particles the Fermion operator is made up from bosons iva the formula

$$\text{Free:} \quad \psi_\sigma^\Omega(r) = \rho_0 e^{-i/\sqrt{2}(\theta_c + \sigma \theta_s)} \; , \tag{12}$$

which gives the Green's function

$$G_{\text{free}} = \frac{1}{\sqrt{r - v_s t + i/\Lambda}} \frac{1}{\sqrt{r - v_c t + \dfrac{i}{\Lambda}}} \quad (v_c = v_s) \; . \tag{13}$$

But we cannot assume that the connection between interacting electrons and the modified bosons obeys (12). The coupling of the two Fermi surfaces which leads to the modified CR means that (12) creates an object which can be thought of as a pseudoelectron, with the suitable backflow caused by the fractional opposite-spin hole which accompanies it, so it describes an exact eigenexcitation of electronlike character moving in the exact ground state. These excitations are analogous to bosonized versions of the exact eigenexcitations of charge $(I_i)$ and spin $(J_\alpha)$ of the Lieb-Wu solution of the 1D Hubbard model. (The discussion here was foreshadowed in Ren's thesis.[12]) These ladders of excitations can be described in terms of appropriate bosons since they have linear energy-momentum relations near zero energy, and these are the bosons which we have derived. But the actual electron operator creates a physical electron, not the pseudoelectrons described by these bosons, and hence must have the backflow compensated out. This leads to the fractional exponents in the Green's function and other correlation functions characteristic of the Luttinger liquid. As in the 1D case (as shown in Ren's thesis) the coefficients may be deduced from conservation laws and from the Luttinger theorem of incompressibility of the Fermi sea in momentum space.

Note that the pseudoelectron has the quantum numbers of a true electron, and in fact it is one of the packet of exact eigenstates created when a true electron is inserted at the appropriate momentum, though with vanishing amplitude as $L \to \infty$. When a real electron is added, a cloud of particle-hole excitations in addition to the two semions is excited, analogous to the cloud of particle-hole excitations which causes the x-ray edge anomaly. This is the backflow. The modified commutation relations of the charge and spin bosons still leave them as a bosonic description of particles which are semions in the sense that two of them make an electron. The transformation which diagonalizes the CR is not modified from the free-particle case, i.e., it is independent of $\eta$.

This is essentially because we maintain Luttinger's theorem of incompressibility as a constraint, so that no net down-spin particles are removed by the scattering process: they are merely redistributed in momentum space, which is the backflow we must now calculate. $\eta/\pi$ particles are displaced from the neighborhood of the scatterer particle at $k\uparrow$, and we must find how they displace the Fermi surface bosons, i.e., how the phases are shifted at the fermi surface. But first we must take into account some consequences of the non-Abelian spin symmetry which we have been ignoring so far.

A key theorem of the bosonization technique follows from the symmetry properties of the states at the Fermi surface. As we stated above, the existence of a Fermi surface implies separate conservation of each component of spin at each point on the Fermi surface. But spin conservation must remain independent of the choice of axes, and we must be able to choose the axes at each point independently. A related requirement is that Kramer's degeneracy of the spin at each point of the fermi surface independently must be maintained. This is not possible if spin at different Fermi points is coupled relevantly as $\omega \to 0$. As is seen in the 1D Hubbard model, this implies that the spin bosons cannot acquire an anomalous dimension, and must retain the same semionic character that they have for free fermions. In our situation, this expresses itself by the observation that our scattering calculation is slightly incomplete. We have not required formal spin rotation invariance [SU(2) symmetry] of the $S$ matrix for scattering, which requires that the phase shift have the form

$$\eta = \eta_c + \eta_s (\sigma \cdot \sigma') \tag{14}$$

and allows for a spin-flip scattering, which we have so far ignored, of half the magnitude $\eta$ of the potential term. This requires the scattering to take place entirely in the singlet channel, rather than the up-down channel, as we have implied in our discussion so far. Our previous picture left us with one spin $k\uparrow$ plus a hole of magnitude $\eta/\pi$ in $k\downarrow$. This left $1 + \eta/\pi\uparrow$ spins, but now we have spin-flip scattering of $\eta/2$ giving $\eta/2\pi$ missing down-spins and $1 - \eta/2\pi$ up-spins or one net spin. Correspond-

ingly, this gives matching currents of up-spin in the scattered channels which leaves us with displacements only of charge, not spin, bosons in the backflow. The comoving hole of magnitude $\eta/\pi$ is now in the charge channel.

In the actual 1D Hubbard model, this theorem is satisfied only to logarithmic accuracy, leading to $(\ln\omega)^{-1}$ and $(\ln q)^{-1}$ corrections to power laws; the relevant coupling constant goes to zero only logarithmically. We expect the same pathology in 2D. But dominant power laws will be correctly determined by bosonization. (All of this was foreshadowed in Haldane's "Luttinger liquid" treatment of the 1D Hubbard model.[13]) When the spin-flip component is taken into account, we now can determine how the phases at the Fermi surface are shifted, specifically when we insert an electron at $\Omega,q$ in order to calculate the one-particle Green's function. The rule is very simple: we calculate the phase shifts we would have expected using naive up-spin down-spin scattering, and replace these by phase shifts in the pure charge channel. Let us first discuss the 1D case, which was worked out by Ren.[12]

In 1D, the amount of charge $\eta/\pi$ which is displaced from the state $k = k_F - q$ appears, half at the left-hand Fermi point and half at the right, i.e., $\eta/2\pi$ at each. These components multiply the Green's function by the factor

$$e^{i\theta_c^r(\eta/2\pi)(1/\sqrt{2})} \, e^{i\theta_c^l(\eta/2\pi)(1/\sqrt{2})} \, ,$$

which gives, in space-time representation, a factor

$$\left[ \frac{1}{(x^2 - v_c^2 t^2)} \right]^{1/4(\eta/2\pi)^2} , \tag{15}$$

which has the maximum exponent $(\frac{1}{2})^2 \times \frac{1}{4} = \frac{1}{16}$, as pointed out by Ren. This gives the famous Fermi-surface smearing exponent $2 \times \frac{1}{16} = \frac{1}{8}$ in the strong-coupling case, and with the strictly local interaction appropriate to the Hubbard model.

These two displacements are the total backflow. The net momentum of the backflow is zero, and the net charge $\eta/\pi$, as it must be.

The situation in 2D is not quite so simple. Again, we recognize that $\eta/\pi$ worth of charge boson—i.e., $\eta/\pi$ enclosed by an internal Fermi surface—has been displaced from the region of momentum $k$. We may calculate the
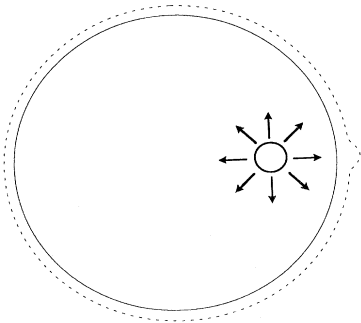


FIG. 1. Dilation of the Fermi surface due to the comoving hole.

displacement of a circular Fermi surface which would result from elastic incompressible deformation of the lattice of $k$ values. (We use a circular FS for illustrative purposes.) This would give us

$$\delta \mathbf{k}' = \frac{\mathbf{k}' - \mathbf{k}}{(k' - k)^2} \frac{\eta}{2\pi^2}$$

and

$$\delta k_F^{(\Omega)} = \frac{\mathbf{k}_F(\Omega)\cdot(\mathbf{k}_F - \mathbf{k})}{(k_F - k)^2} \frac{\eta}{2\pi^2} . \tag{16}$$

See Fig. 1. If $k$ is chosen at $\theta = 0$, and $k = k_F - \epsilon$,

$$\delta k_F(\Omega) \simeq \frac{\epsilon k_F}{\epsilon^2 + k_F^2 \theta^2} \frac{\eta}{2\pi^2} + \frac{\eta}{2\pi^2} \frac{1 - \cos\theta}{2(1 - \cos\theta)}$$

$$= \frac{\eta}{2\pi} \delta(\theta) + \frac{\eta}{(2\pi)^2} . \tag{17}$$

In this case, half of the displacement is in the forward direction, and half is a uniform displacement of the Fermi level—essentially an $s$ wave, equivalent to isotropic potential scattering. This, however, is not quite the whole story. In one dimension the backflow compensated the charge and momentum exactly, since the left- and right-moving pieces were identical. Here, however, we have an uncompensated momentum of the forward-moving wave, $\eta/2\pi \times k_F$. The correct displacement satisfying the Luttinger-Ward theorems is not merely a dilation of the momentum lattice, but a rigid displacement of $-\eta/2\pi k_F$ as well.

The simple uncompressible dilation of the Fermi surface which we postulated in (16) is too simple: the interactions must satisfy momentum as well as particle conservation, and so the backflow must carry no net momentum, as in 1D. The relative $s$-wave channel must carry momentum $-(\eta/2\pi)k_F$, which compensates the extra momentum of the $\delta$-function peak at $\mathbf{k}_F$. This is equivalent to a uniform translation of the Fermi surface, which is a simple unitary transformation (multiplication of all states by a common factor) and does not lead to any anomalous dimensions. On the other hand, the $s$-wave dilation does do so, and the anomalous dimension of the Green's function is, as in 1D, $(\eta/2\pi)^2 \times \frac{1}{2} = \alpha, 0 \leq \alpha \leq \frac{1}{8}$. Another way of describing this part of the backflow is as a Fermi-surface shift proportional to $(1 - 2\cos\theta)$ rather than simply to 1. This is not a scattering in the $p$-wave channel; rather it is more like a "Mossbauer" zero-phonon, coherent recoil of the Fermi sea as a whole.

The form of the Green's function is quite different from 1D: it will look something like

$$G(\mathbf{r},t) \propto \int d\Omega e^{i\mathbf{k}_F(\Omega)\cdot\mathbf{r}}$$

$$\times \left\{ \frac{1}{[\mathbf{r}\cdot\hat{\mathbf{n}}(\Omega) - v_s t]^{1/2}} \right.$$

$$\times \frac{1}{[\mathbf{r}\cdot\hat{\mathbf{n}}(\Omega) - v_c t]^{1/2 + 1/4(\eta/2\pi)^2}} \right\}$$

$$\times \left[ \frac{1}{r - v_c t} \right]^{(\eta/2\pi)^2 \times 1/4} . \tag{18}$$

$\hat{n}(\Omega)$ is the Fermi surface normal unit vector at $\Omega$, and $\cos\theta = \hat{n}(\Omega)\cdot\hat{r}$. The stationary phase will ensure that $G(r,t)$ comes almost entirely from the "patch" $n(\Omega)\|r$.

Experimentally, several hints suggest that $\alpha > \frac{1}{8}$ in fact, in some of the cuprates. We must not be surprised by the parallel-spin interaction also being finite and repulsive, which will enhance the charge-channel backflow without affecting spin properties except to lower $v_s$ further, and make the electrons even less Fermi liquid. For the Hubbard model there is a fixed relation between $\eta_c$ and $\eta_s$ in (14), but in the physical case $\eta$ can be larger.

Most of the physical phenomena which depend on $G$ and other correlation functions can be calculated using the simple homogeneity property

$$G = \frac{1}{t^{1+\alpha}} F\left[\frac{r}{t}\right] .\tag{19}$$

This determines the infrared spectrum in parallel and perpendicular polarizations,[14,15] and the Fermi-surface smearing; a similar property will give the exponent for $1/T_1$. Only angle-resolved photoemission spectroscopy (ARPES) requires the full $G$. This will depend critically on details of the single-particle dispersion and Fermi surface, and so will require a separate investigation.

With (18) we have a principle the asymptotic solution of the 2D electron gas with a local, repulsive interaction. This is expected to be valid in the regions of the phase diagram of the Hubbard model reasonably far from half-filling (where umklapp terms are important and can pin down the charge bosons) and $U \to \infty$ at high density, where ferromagnetic coupling of Landau mean-field type

will possibly be important, and lead to Nagaoka ferromagnetism. Finally, we exclude strong magnetic fields, strong being enough to allow interference after a full cyclotron orbit; i.e., we require $\omega_c \tau \ll 1$ where $\omega_c$ is the cyclotron frequency. Under this condition transverse gauge transformations are simple reparametrizations of the Fermi surface and meaningless; i.e,. the Fermi surface and anyons are mutually incompatible. $\omega_c\tau \gg 1$ destroys the symmetries implicit in the Fermi surface, and causes gaps in the spectrum which are incompatible with bosonization. With $\omega_c\tau < 1$ bosonization is the only gauge theory of the interacting Fermi system; there is no meaningful other.

Khveshchenko has argued that in $\geq 2$ dimensions the equations of motions of the bosons are a very crude approximation valid only for very small $q$ and $\omega$. This is clearly so in our approach, since the $\delta$ function in Eq. (17) is actually of width $q$. We have argued that Chern-Simons types of terms are not important if $\omega_c\tau < 1$, but insofar as charge and spin velocities differ, there can be effects such as those we have postulated in the past caused by mixing of bosons over a finite area of the Fermi surface, when electrons of finite $q = k - k_F$ are excited. Thus the above is a first approximation to a much more complex theory which we do not yet have under control. Nonetheless it seems the only way to proceed.

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