Nonlocal Order Parameters for the 1D Hubbard Model

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We characterize the Mott-insulator and Luther-Emery phases of the 1D Hubbard model through correlators that measure the parity of spin and charge strings along the chain. These nonlocal quantities order in the corresponding gapped phases and vanish at the critical point $U_c = 0$, thus configuring as hidden order parameters. The Mott insulator consists of bound doublon-holon pairs, which in the Luther-Emery phase turn into electron pairs with opposite spins, both unbinding at U_c. The behavior of the parity correlators is captured by an effective free spinless fermion model.

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The Hubbard model and its extensions have been widely used to investigate the behavior of strongly correlated electrons in several condensed-matter systems ranging from Mott insulators (MI) to high-T_c superconducting materials. Recently, progress in ultracold gas experiments that use fermionic atoms trapped in optical lattices has opened the way to the direct simulation of the Hubbard model and the observation of the predicted MI phase [1]. Since the Mott transition in one dimension (1D) is known to be of Berezinskii-Kosterlitz-Thouless (BKT) type [2], the order parameter cannot be *local*; instead, the transition point should correspond to the vanishing of some topological order. On general grounds, it was shown that the vanishing of conductivity can be related to the nonvanishing of nonlocal quantities [3–6]. Nevertheless, an order parameter for solely the MI phase has not yet been identified. Progress has been achieved in the related field of the bosonic Hubbard models, where the correspondence of the bosonic system with spin-1 Hamiltonians at low energy near integer filling has allowed characterization in 1D MI and Haldane insulator phases by means of nonlocal string parameters [7–10]. One of these is related to the parity correlator $O_P(r) = \langle e^{2i\pi\sum_{j=i}^{i+r} S_{z,j}}\rangle$, with $S_{z,i} = \frac{1}{2}(n_i - \nu)$ measuring the parity of the deviation of the occupation number n_i with respect to the filling ν in a string starting from the site i, ending to the site $i + r$. The nonvanishing value of the parity parameter $O_P = \lim_{r\to\infty} O_P(r)$ in the insulating phase has been observed with *in situ* imaging in experiments on ultracold bosonic ^{87}Rb atoms [11].

In this Letter, we show that two parity string correlators work as order parameters for the two gapped phases of the fermionic Hubbard model in 1D. In this case, the expected role of antiferromagnetic (AFM) correlations has so far driven the attention mainly to the study of Haldane-type string correlators; these were found to vanish algebraically, together with $O_P(r)$ in the Luttinger liquid regime [12]. On the other hand, at half-filling in the large Coulomb repulsion limit the Hubbard Hamiltonian is known to reduce to the AFM Heisenberg Hamiltonian, for which the parity string correlator is identically 1, the wave function being frozen to the sector with only one electron per site. At finite Coulomb repulsion instead, in the MI phase the number of doubly occupied sites (doublons) and empty sites (holons) is nonvanishing (as also observed experimentally [1]). Hence, an appropriate parity parameter should characterize the transition from the Heisenberg to the Luttinger liquid limit, marking the existence of the whole MI phase.

The local four-dimensional vector space on which an electron Hamiltonian acts is typically generated by application to the vacuum operators forming a su(4) algebra, with three Cartan generators. Consequently, we can introduce two independent parity correlators $O_P^{(\nu)}$, defined as

$$O_P^{(\nu)}(r) = \left\langle e^{2i\pi\sum_{j=i}^{i+r} S_{z,j}^{(\nu)}}\right\rangle, \tag{1}$$

with index $\nu = c, s$, namely, the "charge" and "spin" generalizations of the parity correlator $O_P(r)$. Here, $S_{z,i}^{(\nu)}$ are the spin and pseudospin operators defined respectively as $S_{z,i}^{(s)} = \frac{1}{2}(n_{i,\uparrow} - n_{i,\downarrow})$ and $S_{z,i}^{(c)} = \frac{1}{2}(n_{i,\uparrow} + n_{i,\downarrow} - 1)$, with $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, $\sigma = \uparrow, \downarrow$, $c_{i\sigma}^\dagger$ creating a fermion at site i with spin σ. By means of bosonization and density matrix renormalization group (DMRG) analysis, we will show that each $O_P^{(\nu)}$ orders in the corresponding gapped phase: MI for $\nu = c$, with open charge gap, and Luther-Emery (LE) for $\nu = s$, with open spin gap. The $O_P^{(\nu)}$ vanish with the gap at the BKT transition point where the correlation length becomes infinite. Notice that the two parameters collapse into a single one in the spin-1 case.

The Hubbard model is described by the Hamiltonian

$$\mathcal{H} = -\sum_{i\sigma}(c_{i\sigma}^\dagger c_{i+1,\sigma} + c_{i+1,\sigma}^\dagger c_{i\sigma}) + U\sum_i n_{i\uparrow}n_{i\downarrow} \tag{2}$$

where the overlap integral U gives the on-site contribution of Coulomb repulsion and energy is expressed in units of the tunneling amplitude.

The bosonized form of the half-filled Hubbard Hamiltonian at low energy is known to give rise to two

continuum models separately describing the spin and charge sectors [2]. The latter is described by the Hamiltonian

$$H_c = \int dx \left\{ \frac{v_c}{2\pi} \left[K_c \pi \Pi_c^2 + \frac{1}{K_c} (\partial_x \Phi_c)^2 \right] - \frac{2U}{(2\pi\alpha)^2} \cos(\sqrt{8}\Phi_c) \right\} \quad (3)$$

with

$$v_c = v_F \left(1 + \frac{U}{\pi v_F}\right)^{1/2}, \qquad K_c = \left(1 + \frac{U}{\pi v_F}\right)^{-1/2}. \quad (4)$$

Here, Φ_c is the compactified boson describing the charge excitations with velocity v_c, and $\Pi_c = \partial_x \Theta_c/\pi$ is its conjugate momentum (α is a cutoff). At the BKT transition point $U = 0$, we have $K_c = 1$. The bosonic field in the spin sector Φ_s is governed by equations that can be obtained from Eqs. (3) and (4) by replacing $U \to -U$ and $c \to s$. The spin-charge transformation $c_{j\downarrow} \to (-1)^j c_{j\downarrow}^\dagger$, which implies $S_{z,j}^{(c)} \to S_{z,j}^{(s)}$, in the present bosonization analysis corresponds simply to the change $\Phi_c \leftrightarrow \Phi_s$. In fact, we have used the continuum prescriptions used in Ref. [2] where $S_z^{(s)}(x) = \partial_x \Phi_s(x)/(\sqrt{2}\pi)$ and $S_z^{(c)}(x) = \partial_x \Phi_c(x)/(\sqrt{2}\pi)$.

For $U > 0$, we get $K_s > 1$: the cosine term in H_s is (marginally) irrelevant, and the spin excitations are gapless and governed by an ordinary Gaussian model. Meanwhile, $K_c < 1$, and a charge gap is generated by the relevant cosine term in H_c. As a consequence, the field Φ_c is pinned in one of the classical minima of the cosine term, i.e., $\Phi_c = (2\pi m)/\sqrt{8}$, $m \in \mathbb{Z}$, while Φ_s does not order. For $U < 0$, just the same occurs with inverted roles $\Phi_c \leftrightarrow \Phi_s$. In the continuum limit, one can realize that the parity operators become [9,13]

$$O_P^{(\nu)}(r) \approx \langle \cos[\sqrt{2}\Phi_\nu(r)] \cos[\sqrt{2}\Phi_\nu(0)] \rangle.$$

Hence, in the MI phase at $U > 0$, $O_P^{(c)}$ turns out to be nonvanishing. In the $U < 0$ case instead the LE phase is characterized by nonzero $O_P^{(s)}$. The two Haldane-type string correlators

$$O_S^{(\nu)}(r) = \left\langle S_{z,i}^{(\nu)} e^{2i\pi \sum_{j=i}^{i+r} S_{z,j}^{(\nu)}} S_{z,i+r}^{(\nu)} \right\rangle$$

give instead $O_S^{(\nu)}(r) \approx \langle \sin[\sqrt{2}\Phi_\nu(r)] \sin[\sqrt{2}\Phi_\nu(0)] \rangle$, where the same argument suggests that these are both asymptotically vanishing in the two gapped phases. From the above derivation, we can conjecture that a necessary and sufficient condition for having an asymptotically nonvanishing charge (spin) parity correlator in the Hubbard model is the opening of a gap in the charge (spin) sector, so that $O_P^{(\nu)}$ do configure as order parameters for the gapped phases of the Hubbard model.

Below, we support our previous argument providing a quantitative estimation of the parity string parameter in the MI phase. This is achieved by means of numerical analysis using the DMRG algorithm on finite size chains with periodic boundary conditions (PBCs). The analysis requires very precise and reliable data; in fact, the computing effort is significant due to both the slowdown caused by PBCs and the high sensitivity of the correlations contained in $O_P^{(\nu)}(r)$ with respect to numerical errors. Hence, we have chosen to consider chain sizes from $L = 10$ to $L = 50$ and 1024 DMRG states. The curves of $O_P^{(c)}(r)$ plotted in Fig. 1 for $L = 50$ clearly make evident a fast convergence to the asymptotic values for high interactions as well as a progressive increase of the parity order with U. The presence of two sequences for even and odd r that tend toward the same asymptotic limit also signals that the spin parity correlator $O_P^{(s)}(r) = (-1)^r O_P^{(c)}(r)$ has a uniform part $[O_P^{(s)}(2r+1) + O_P^{(s)}(2r)]/2$ that goes smoothly to zero for $U > 0$. The opposite mechanism holds for negative values of the interaction.

Exactly at $U = 0$ both parity orders are absent and $O_P^{(c)}(r) = O_P^{(s)}(r)$ as required by the spin-charge symmetry. Here, an analytic calculation of $O_P^{(\nu)}(r)$ can be performed independently for both spin species by using the Wick theorem and evaluating Toeplitz determinants. An estimation of the asymptotic behavior gives $O_P^{(c)}(r) \sim r^{-1}$ at $U = 0$ [14].

We have explicitly evaluated the order parameter $O_P^{(c)}$ in the MI phase and plotted it in Fig. 2 for several values of U. The asymptotic values have been extrapolated from the finite-size scaling of the quantity $O_P^{(c)}(L/2)$ in a periodic chain of length L. For the fits, we have made use of functions $O_P(r) = O_P + Ar^{-\gamma} e^{-r/\xi}$ obtaining a good convergence. Interestingly, as evidenced in the inset of Fig. 2, for small U we get $\gamma = 1$ and $A > 0$, and for strong

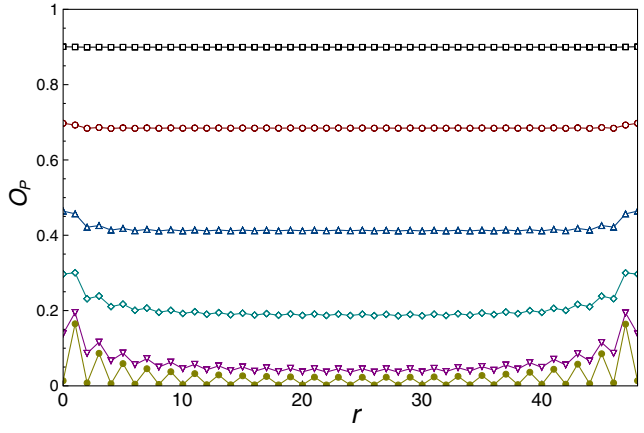

FIG. 1 (color online). Parity correlator $O_P^{(c)}(r)$ for a periodic chain with $L = 50$ as a function of the string length r. The sequences of data refer to $U = 0.1$, 1.0, 2.0, 3.0, 5.0, 10.0 (in ascending order).

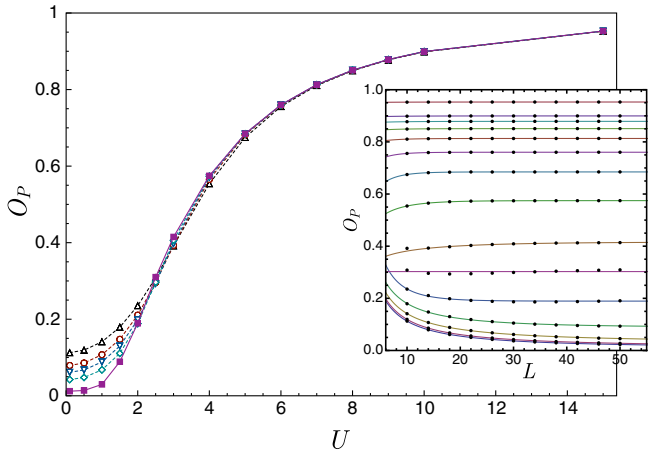

FIG. 2 (color online). Charge parity order parameter measured at half chain $O_P^{(c)}(L/2)$ as a function of the local interaction U. We have considered PBCs and finite chain lengths from $L = 10$ to $L = 50$ in steps of 4, a sequence for which the ground state of the Hubbard model is unique. We have plotted the curves for $L = 10$ (up triangles), $L = 14$ (circles), $L = 18$ (down triangles), $L = 26$ (rhombuses). The filled squares represent the finite size scaling values to $L = \infty$ obtained by the fits shown in the inset.

interactions we obtain $\gamma = 1/2$ and $A < 0$; for intermediate values, the best fit seems to be a combination of the two functions.

The nonvanishing of $O_P^{(c)}$ implies the existence of bound doublon-holon pairs (see Ref. [9]); their correlation length increases by decreasing U becoming infinite at the transition, when pairs finally unbind. The quasi-long-range AFM order of the MI phase suggests that such pairs are diluted in an AFM background of single electrons. The spin-charge transformation that maps positive U Hamiltonian at half-filling into negative U case at zero magnetization allows one to extend the same type of analysis to the LE phase, which is then characterized at any filling by bound pairs of single electrons with opposite spins.

On the basis of the above scenario, we construct an approximation scheme that aims at isolating the relevant degrees of freedom (charges) to describe the actual role of $O_P^{(\nu)}$ in the Hubbard model. Since the operator $e^{i\pi n_j} = (-1)^{n_j}$ changes sign whenever the site j is singly occupied, no matter its spin orientation, we choose to represent the original electronic creation operators $c_{i\sigma}^\dagger$ in terms of a spinless fermion $f_i^\dagger$ and Pauli operators σ_i^a, $a = x, y, z$ acting on a spin part. The mapping, schematized in Table I, is identified by the unitary transformation

TABLE I. Mapping from electrons to spinless fermions and σ spins.

Spinful fermion	$\|0\rangle$	$\|\uparrow\rangle$	$\|\downarrow\rangle$	$\|\uparrow\downarrow\rangle$
Spinless fermion $\otimes$ σ spin	$\|0\rangle\|+\rangle$	$\|1\rangle\|+\rangle$	$\|1\rangle\|-\rangle$	$\|0\rangle\|-\rangle$

$$c_{i\uparrow}^\dagger = c_{i\uparrow}^\dagger(1 - n_{i\downarrow}) + c_{i\uparrow}^\dagger n_{i\downarrow} = f_i^\dagger P_i^+ + (-1)^i f_i P_i^-,$$
$$c_{i\downarrow}^\dagger = c_{i\downarrow}^\dagger(1 - n_{i\uparrow}) + c_{i\downarrow}^\dagger n_{i\uparrow} = [f_i^\dagger - (-1)^i f_i]\sigma_i^-,$$

with $P_i^\pm = \frac{1 \pm \sigma_i^z}{2}$. Interestingly, the interaction term for the c fermions simply becomes a chemical potential shift for f fermions, namely, $U\sum_i n_{i\uparrow}n_{i\downarrow} = U(N - \sum_i n_i^f)/2$, where $N = \sum_{i,\sigma} n_{i\sigma}$. According to this picture, the spin and pseudospin operators are $\mathbf{S}_j^{(s)} = f_j^\dagger f_j \boldsymbol{\sigma}_j$ and $\mathbf{S}_j^{(c)} = f_j f_j^\dagger \boldsymbol{\sigma}_j$; conversely, we have $\boldsymbol{\sigma}_j = \mathbf{S}_j + \mathbf{J}_j$.

After the mapping, the model in Eq. (2) becomes

$$\mathcal{H} = -\sum_{\langle ij \rangle}\Big[f_i^\dagger f_j Q_{ij} - 2(-1)^i f_i^\dagger f_j^\dagger R_{ij} + \text{H.c.}\Big] + \frac{U}{2}\Big(N - \sum_i f_i^\dagger f_i\Big), \tag{5}$$

where $Q_{ij} = (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + 1)/2$ is just the swap operator in the σ-spin state and $R_{ij} = (1 - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)/4$ is the projector onto the singlet. Notice that Eq. (5) is invariant under global σ-spin rotations.

The form (5) for the Hubbard model holds in arbitrary dimension, and its terms are quadratic with respect to f fermions. Since $O_P^{(\nu)}$ can be entirely expressed in terms of f_i, a possible strategy consists of tracing out the σ spins by some mean-field approximation. In fact, by exploiting the symmetries of the Hubbard model one can easily realize that $\langle Q_{ij} \rangle = 1/2$ is an exact identity on the states with nonvanishing hopping term in (5). Moreover, we set the parameter $\alpha \equiv \langle R_{ij} \rangle$ in a phenomenological way by equating the ground-state (GS) energy obtained from the spinless quadratic model with the exact energy coming from the Bethe-ansatz solution [15]. Within this approximation, Eq. (5) is diagonalized in Fourier space (see Supplemental Material [16]), obtaining

$$H = \sum_{k \in \text{BZ}} \Lambda_k \Big[\eta_k^\dagger \eta_k - \frac{1}{2}\Big] + \frac{U(2N - L)}{4},$$

with spectrum $\Lambda_k = -\cos k + \sqrt{16\alpha^2 \cos^2 k + U^2/4}$, and where η_k are the new fermionic modes. In the thermodynamical limit (TL), the energy density e_{GS} at half-filling $\nu = 1$ is given by $e_{\text{GS}} = \frac{U}{4} - \frac{1}{2\pi}\int_{-\pi/2}^{\pi/2} dk \sqrt{16\alpha^2 \cos^2 k + U^2/4}$. It is interesting to observe that the model is gapless only for $U = 0$, where for $\alpha = 1$ e_{GS} assumes the exact value of the noninteracting case. For $U > 0$, the number of singly occupied states ν_f is increasing and the pair-singlet states start to interact.

We are interested in calculating the parity operator $O_P^{(c)}(r) = \langle e^{i\pi \Sigma_{j=i}^{i+r}(n_j^f - 1)} \rangle$ that can be rewritten as

$$O_P^{(c)}(r) = \left\langle \prod_{j=i}^{i+r} (2f_j^\dagger f_j - 1) \right\rangle = \left\langle \prod_{j=i}^{i+r} A_j B_j \right\rangle,$$

having defined $A_j = (f_j^\dagger + f_j)$ and $B_j = (f_j - f_j^\dagger)$. By use of the Wick theorem, $O_P^{(c)}(r)$ can be expressed as a determinant [17]

$$O_P^{(c)}(r) = \begin{vmatrix} G_0 & G_1 & G_2 & \cdots & G_{i,i+r} \\ -G_1 & G_0 & -G_1 & \cdots & \\ G_2 & G_1 & G_0 & \cdots & \\ \vdots & \vdots & \vdots & \ddots & \cdots \\ G_{i+r,i} & & & \vdots & G_0 \end{vmatrix} = \det(\mathbf{G}). \quad (6)$$

where $\mathbf{G}$ is a block Toeplitz matrix of dimension $(r+1) \times (r+1)$, whose entries are the one-body correlation functions $G_r = \langle (f_j^\dagger - f_j)(f_{j+r}^\dagger + f_{j+r}) \rangle$, whose expressions in the TL are

$$G_r = \begin{cases} \frac{U}{2\pi} \int_0^\pi dk \frac{\cos(kr)}{\sqrt{16\alpha^2 \cos^2(k) + U^2/4}}, & r \text{ even} \\ (-1)^j \frac{4\alpha}{\pi} \int_0^\pi dk \frac{\cos(kr)\cos(k)}{\sqrt{16\alpha^2 \cos^2(k) + U^2/4}}, & r \text{ odd} \end{cases}$$

with the property that $G_0 = 2\nu_f - 1$, $G_r = 2\mathrm{Re}(\langle f_j^\dagger f_{j+r} \rangle)$ for r even, and $G_r = 2\mathrm{Re}(\langle f_j^\dagger f_{j+r}^\dagger \rangle)$ for r odd. The blocks in (6) are of size 2×2. We must distinguish the cases of r even or odd, since they give rise to two different sequences. In particular, here we stick to the case r odd, where the block matrix is of even dimension.

The analytical calculation of $O_P^{(c)}$ in the TL for some values of U in the f-fermion approximation yields to the curve plotted in Fig. 3, providing evidence for the expected nonvanishing of the charge parity order for $U > 0$. The parameter α has been determined by requiring $e_{\mathrm{GS}}(U, \alpha) = e_{\mathrm{ex}}(U)$, where e_{ex} is the exact result [15]. Remarkably, such equality admits a solution for every U, which belongs to a narrow interval below $\alpha = 1$, as shown in the inset of Fig. 3. This means that in the pair-creation processes in Eq. (5), the σ-spin state is very close to the singlet. In the limit $U \gg 1$, the energy becomes $e_{\mathrm{GS}}(\alpha) \approx -4\alpha^2/U$ that gives $\alpha(U \to \infty) = \sqrt{\log 2} \approx 0.83$, by comparison with the energy density of the Heisenberg model coming from the large-U expansion of the Hubbard model at $\nu = 1$. The result for $O_P^{(c)}$ is also quantitatively in accordance with the DMRG data in the large U region, where our assumptions on the AFM nature of short-ranged correlations [18] are more justified.

In conclusion, our work unveils that two (charge and spin) parity string correlators are the order parameters for the gapped phases of the 1D Hubbard model. In the bosonization approach, these are found to be asymptotically

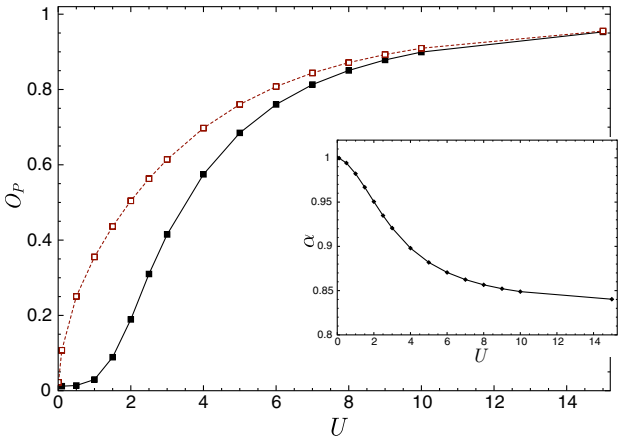

FIG. 3 (color online). Parity order $O_P^{(c)}$ calculated according to Eq. (6) as a function of U (dashed line) in the MI phase of the effective model (5) with α as in the inset figure, determined by tuning the spinless fermion energy to the exact Hubbard value. The results are compared with the numerical curve (continuous line) obtained for the Hubbard model and shown in Fig. 2.

finite only in the corresponding gapped MI and LE phases and vanish with the gap at the BKT transition point. The result is cleanly confirmed by DMRG numerical analysis. The quantity $O_P^{(c)}$ characterizes the MI as a phase in which bound pairs of doublons and holons move in an AFM background of single electrons. In the LE regime, the roles of doublons and holons and that of up and down electrons are interchanged. The picture allows us to derive an effective free spinless fermion model that correctly captures the presence of nonlocal order and its vanishing at the transition. The spinless model is exact in the limit of large U values, thus complementing the standard strong-coupling description with the t-J model.

The parity order is suitable for experimental detection by high-resolution imaging [11] in ultracold Fermi gases. Some of the features described here could possibly persist in two dimensions, where the localization of bound pairs could take place along one-dimensional stripes. The scenario is quite suggestive also from the perspective of high-T_c materials, where the presence of bound doublon-hole pairs in the undoped insulator could play a role upon doping in the onset of the superconducting phase. In fact, the latter could be seen here as the LE phase in which doublons freely move in a sea of correlated pairs of single electrons with opposite spins.

The present analysis could be further exploited to extended Hubbard models [3,19,20], to investigate the presence of these types of topological order in other gapped phases. For instance, the presence of both charge and spin gaps in principle may give rise to four different phases, depending on the vanishing or nonvanishing values of the two $O_P^{(\nu)}$'s. Work is in progress along these lines.

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