Hidden Quasi-One-Dimensional Superconductivity in $Sr₂RuO₄$

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We show that the interplay between spin and charge fluctuations in $Sr_2RuO₄$ leads unequivocally to triplet pairing which has a hidden quasi-one-dimensional character. The resulting superconducting state spontaneously breaks time-reversal symmetry and is of the form $\Delta \sim (p_x + ip_y)\hat{z}$ with sharp gap minima and a *d* vector that is only *weakly* pinned. The superconductor lacks robust chiral Majorana fermion modes along the boundary. The absence of topologically protected edge modes could explain the surprising absence of experimentally detectable edge currents in this system.

Introduction.—Sr₂RuO₄ is a layered perovskite material, isostructural to the hole-doped 214 family of cuprate superconductors. Below $T \sim 50 K$, it exhibits Fermi liquid behavior and undergoes a superconducting transition at $T_c = 1.5 K$. There is compelling experimental evidence which suggests that this superconducting state has odd parity [\[1,](#page-3-0)[2](#page-3-1)] and spontaneously breaks time-reversal [[2](#page-3-1)[–4\]](#page-3-2) symmetry. One of the simplest superconducting gap functions which meets both of these requirements is the chiral p-wave state, $\Delta(p) \propto (p_x + ip_y)\hat{z}$, a quasi-twodimensional version of superfluid 3 He-A [\[5,](#page-3-3)[6](#page-3-4)].

In its simplest form, this chiral pairing gives rise to a topological superconductor: all Bogoliubov quasiparticle excitations are gapped in the bulk whereas topologically protected chiral Majorana fermion modes exist at the edge of the system and in vortex cores [[7\]](#page-3-5). These modes are robust against all perturbations, including disorder, so long as the BCS pairing gap in the bulk remains finite. In addition, spontaneous supercurrents are expected at sample edges and domain walls [\[8](#page-3-6),[9](#page-3-7)].

However, scanning SQUID imaging studies [\[10\]](#page-3-8) have revealed that edge currents of the expected magnitude are *not* found in Sr_2RuO_4 . Moreover, low temperature power laws in the electronic specific heat [[11](#page-3-9)] and the nuclear spin relaxation $1/T_1$ [\[12\]](#page-3-10) suggest that this material is not a simple chiral superconductor, which would exhibit exponentially activated behavior in both of these quantities. The form of the superconducting order parameter which accounts for all of the observed phenomena remains unknown. Resolution of this puzzle could come from a careful consideration of the normal state properties, which are known with unprecedented detail [\[13,](#page-3-11)[14](#page-3-12)]. The Fermi surface of $Sr_2RuO₄$ consists of 3 sheets, denoted α , β , γ [\[13](#page-3-11)[,14\]](#page-3-12). The α and β sheets are hole and electron pockets respectively; they are comprised primarily of the Ru d_{xz} , d_{yz} orbitals which form quasi-one-dimensional bands. The γ sheet is composed mainly of the Ru d_{xy} orbital, which forms a quasi-two-dimensional band. A variety of experiments have shown that the system behaves as a quasi-twodimensional Fermi liquid with considerable effective mass enhancements [[14](#page-3-12)]. Therefore, it is likely that electron

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correlations play a significant role in influencing the pairing mechanism of this system.

In this Letter, we present a microscopic theory of superconductivity in $Sr₂RuO₄$. Using a simple extension of a recently developed weak-coupling analysis of the Hubbard model [[15](#page-3-13)], we show that the dominant superconducting instability is in the triplet channel and occurs on the quasi-1D Fermi surfaces of $Sr₂RuO₄$. The resulting superconducting state spontaneously breaks time-reversal symmetry. It exhibits nodelike behavior since it possesses points on the Fermi surface where the gap is parametrically small. It supports Andreev bound states at domain walls and at the edges of the system. However, it is a topologically trivial superconductor without chiral Majorana fermion edge modes.

Microscopic model.—We consider a simple Hamiltonian with three bands derived from the Ru t_{2g} orbitals

$$
H = H_0 + U \sum_{i\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} + \frac{V}{2} \sum_{i,\alpha \neq \beta} n_{i\alpha} n_{i\beta} + \delta H. \tag{1}
$$

Here, we introduce vector indices such that $\alpha = x$, y, and z, refer, respectively, to the Ru d_{xz} , d_{yz} and d_{xy} orbitals, $n_{i\alpha\sigma}$ is the density of electrons having spin σ at position i in orbital α and $n_{i\alpha} = \sum_{\sigma} n_{i\alpha\sigma}$. The strength of the repulsive interaction between two electrons on like (distinct) sive interaction between two electrons on like (distinct) orbitals at the same lattice site is given by $U(V)$. $H_0 = \sum_{\alpha} \sum_{\vec{k}\sigma} (\epsilon_{\alpha\vec{k}}^0 - \mu) c_{\vec{k}\alpha\sigma}^{\dagger} c_{\vec{k}\alpha\sigma}$ is the dominant intraorbital kinetic energy and gives rise to 3 decoupled energy bands at the Fermi level as shown in Fig. [1](#page-1-0). Here, we make use of the following tight-binding parametrization:

$$
\epsilon_{x(y)}^0(\vec{k}) = -2t \cos k_{x(y)} - 2t^{\perp} \cos k_{y(x)} \n\epsilon_z^0(\vec{k}) = -2t'(\cos k_x + \cos k_y) - 4t'' \cos k_x \cos k_y
$$
\n(2)

where we take $(t, t^{\perp}, t', t'', \mu) = (1.0, 0.1, 0.8, 0.3, 1.0)$
[16.17] The quantity δH represents smaller terms such [\[16](#page-3-14)[,17\]](#page-3-15). The quantity δH represents smaller terms such as longer range hopping and spin orbit coupling (SOC) which mix the distinct orbitals. It plays a relatively minor role in determining the superconducting transition temperature. However, δH plays a crucial role in selecting a

FIG. 1 (color online). Tight-binding Fermi surface for the noninteracting Hamiltonian H_0 . Hybridizations among different orbitals are neglected in the solid curve and are included in the dashed curve.

superconducting state which breaks time-reversal symmetry, as will be discussed below. When $\delta H = 0$, the noninteracting susceptibilities of the normal state are separate functions for each orbital:

$$
\chi_{\alpha}(\vec{q}) = -\int \frac{d^2k}{(2\pi)^2} \frac{f(\epsilon_{\alpha, \vec{k} + \vec{q}}) - f(\epsilon_{\alpha, \vec{k}})}{\epsilon_{\alpha, \vec{k} + \vec{q}} - \epsilon_{\alpha, \vec{k}}}
$$
(3)

where $f(\epsilon)$ is the Fermi function. Since the quasi-twodimensional band is almost circular with a radius k_f^{2d} , its susceptibility is nearly constant: $\chi_z \approx 1/4\pi t'$ for $q <$ $2k_f^{2d}$. In contrast, the quasi-1D bands have susceptibilities that are peaked at $\vec{q}_x = (2k_f^{1d}, \pi)$ and $\vec{q}_y = (\pi, 2k_f^{1d})$ for the x and y orbitals respectively. It is the structure of χ the x and y orbitals, respectively. It is the structure of χ_x and χ ^v which gives rise to the incommensurate spin fluctuations in the material [\[18\]](#page-3-16).

Since the superconductivity in $Sr₂RuO₄$ evolves out of a Fermi liquid and $T_c \ll E_f$, it is reasonable to carry out a weak-coupling analysis which treats the limit $U, V \ll W$ where W is the bandwidth. In this limit, superconductivity is the only instability of the Fermi liquid, and it can be treated in an asymptotically exact manner via a two-stage renormalization group analysis [[15\]](#page-3-13). In the first stage, high energy modes are perturbatively integrated out above an unphysical cutoff, and an effective particle-particle interaction in the Cooper channel is derived:

$$
\Gamma_s(\hat{k}, \hat{q}, \alpha) = U + U^2 \chi_\alpha(\hat{k} + \hat{q}) - 2V^2 \sum_{\beta \neq \alpha} \chi_\beta(\hat{k} - \hat{q})
$$

$$
\Gamma_t(\hat{k}, \hat{q}, \alpha) = -U^2 \chi_\alpha(\hat{k} - \hat{q}) - 2V^2 \sum_{\beta \neq \alpha} \chi_\beta(\hat{k} - \hat{q})
$$
 (4)

where $\Gamma_a(\hat{k}, \hat{q}, \alpha)$ ($a = s$ or t) is the effective interaction in the singlet (triplet) channel. In the second stage, the reporthe singlet (triplet) channel. In the second stage, the renormalization group flows of these effective interactions are computed and the superconducting transition temperature is related to the energy scale at which an effective interaction grows to be of order 1:

$$
T_c \sim We^{-1/|\lambda_0^{(a,\alpha)}|} \tag{5}
$$

where $\lambda_0^{(a,\alpha)}$ is the most negative eigenvalue of the matrix

$$
g_{\hat{k},\hat{q}}^{(a,\alpha)} = \sqrt{\frac{\bar{v}_f}{v_f(\hat{k})}} \Gamma_a(\hat{k},\hat{q},\alpha) \sqrt{\frac{\bar{v}_f}{v_f(\hat{q})}}
$$
(6)

with \hat{k} and \hat{q} constrained to lie on the Fermi surface of band α . The pair wave function in the superconducting state is proportional to the associated eigenfunction [\[15\]](#page-3-13).

The values of $\lambda^{(a,\alpha)}$, obtained by numerical diagonaliza-tion, are presented in Fig. [2.](#page-1-1) When $V = 0$, the two dimensional ζ band has its dominant pairing instability in the singlet $d_{x^2-y^2}$ channel and a substantially lower pairing
strength in the triplet p weves abound. By contrast, the strength in the triplet p -wave channel. By contrast, the pairing tendencies of the x and y bands are stronger, and exhibit a close competition between singlet and triplet pairing [\[19\]](#page-3-17). When $V > 0$, only triplet pairing in the quasi-one-dimensional bands is enhanced. Since the solutions with weaker pairing strengths have exponentially smaller transition temperatures in the weak-coupling limit, the effect of subdominant orders is negligible. Thus, in the asymptotically weak-coupling limit, the dominant superconducting instability occurs in the quasi-one-dimensional bands in the spin-triplet channel. For $V > 0$, triplet pairing in the x and y bands is enhanced by virtual charge fluctuations occurring in the z band. This conclusion is robust against a rather large range of quantitative changes of the band parameters [[21](#page-3-18)]. The triplet pair wave function

$$
\Psi_{\alpha}(\vec{k}) = i[\vec{d}_{\alpha}(\vec{k}) \cdot \vec{\sigma}\sigma^{\gamma}], \qquad \alpha = x, y \tag{7}
$$

is specified by the complex vector $\vec{d}_{\alpha}(\vec{k})$ in spin space. In secondgeneral, the real and imaginary parts of \vec{d}_{α} are independent real vectors, and the net spin magnetization of band α is $\vec{M}_{\alpha} \propto \vec{d}_{\alpha}^* \times \vec{d}_{\alpha}$. However, in weak coupling, only "unitary
states " i.e., states with $\vec{M}_{\alpha} = \vec{0}$ need be considered, so \vec{d}_{α} states," i.e., states with $\vec{M}_{\alpha} = \vec{0}$, need be considered, so \vec{d}_{α}
can be expressed, up to a phase, as a real "gan function" can be expressed, up to a phase, as a real ''gap function'' times a real unit vector Ω_{α} :

$$
\vec{d}_{\alpha}(\vec{k}) = \Delta_{\alpha}(\vec{k}) e^{i\theta_{\alpha}} \hat{\Omega}_{\alpha}.
$$
 (8)

FIG. 2 (color online). Pairing eigenvalues as a function of V/U for the band structure parameters quoted in the text. The strongest pairing strengths occur among the quasi-1D $\{\alpha, \beta\}$ bands.
There is a near degeneracy of the singlet and triplet eigenvalues There is a near degeneracy of the singlet and triplet eigenvalues for $V = 0$, but with $V > 0$, the quasi-1D triplet state is the dominant superconducting configuration.

Figure [3\(a\)](#page-2-0) shows the sign of $\Delta_{x}(\vec{k})$ on the xz Fermi surface. In addition to having odd parity, the wave function has two point nodes on the Fermi surface near $k_y = \pm \pi/2$ and is well approximated by $\Delta_x(\vec{k}) \approx \Delta_0 \sin k_x \cos k_y$, and $\Delta_{v}(\vec{k}) \approx \Delta_0 \sin k_v \cos k_x$ on the yz Fermi surface. For $\delta H =$ 0, $\hat{\Omega}_x$, $\hat{\Omega}_y$, θ_x and θ_y are undetermined.

Effect of small interactions.—Next, we consider the effect of including mixing among the different orbitals:

$$
\delta H = \sum_{\vec{k}\sigma} [g(\vec{k}) c_{\vec{k},x,\sigma}^{\dagger} c_{\vec{k},y,\sigma} + \text{H.c.}] + \eta \sum_{\alpha,\beta} \sum_{\sigma\sigma'} \sum_{\vec{k}} c_{\vec{k},\alpha,\sigma}^{\dagger} c_{\vec{k},\beta,\sigma'} \vec{\ell}_{\alpha\beta} \cdot \vec{\sigma}_{\sigma\sigma'} \qquad (9)
$$

where $g(\vec{k}) = -2t'' \sin k_x \sin k_y$, the second quantity above
is the SOC- and the angular momentum operators are exis the SOC, and the angular momentum operators are expressed in terms of the totally antisymmetric tensor as $\ell_{\alpha\beta}^a = i\epsilon_{a\alpha\beta}$. Recent studies have produced the estimates $\ell_{\alpha\beta}^a = 0.1$ t and $\pi \approx 0.1$ t [16.22] $t'' \approx 0.1t$ and $\eta \approx 0.1t$ [[16](#page-3-14),[22](#page-3-19)].
There are several important of

There are several important qualitative effects of including these additional terms in the Hamiltonian: (1) Nonzero t'' or η pins the relative phase, $\theta_x - \theta_y$, and relative orientation, $\hat{\Omega}_x \cdot \hat{\Omega}_y$ of the d vectors. (2) Nonzero η defines a preferred ordering direction for Ω_a . (3) The nodes on the xz and yz Fermi surfaces are gapped, although the gap is parametrically small for small δH . To understand the role of δH in selecting among the large number of possible ordered phases, it is simplest to consider the Landau free energy $\mathcal F$ to low order in powers of the order parameter which is a valid approximation near T_c . Since any order induced on the z band is slaved to the primary order on the x and y bands, we keep explicitly only $\alpha = x$ and y, in which case

$$
\mathcal{F} = \sum_{\alpha} [r|\vec{d}_{\alpha}|^2 + u|\vec{d}_{\alpha}|^4 + \gamma |\vec{d}_{\alpha}^* \times \vec{d}_{\alpha}|^2] + a_1[|d_x^z|^2
$$

+ $|d_y^z|^2] + a_2[|d_x^x|^2 + |d_y^y|^2] + v_1|\vec{d}_x|^2|\vec{d}_y|^2$
+ $v_2|\vec{d}_x \cdot \vec{d}_y|^2 + J_1|\vec{d}_x^* \cdot \vec{d}_y + \vec{d}_y^* \cdot \vec{d}_x|^2$
+ $J_2|\vec{d}_x^* \times \vec{d}_y + \vec{d}_y^* \times \vec{d}_x|^2$ (10)

where the terms in the first line survive the $\delta H \rightarrow 0$ limit, $a_i \sim \mathcal{O}(\eta^2/t^2)$, and v_i and J_i have contributions of order $(\eta/t)^2$ and $(t''/t)^2$. To quadratic order in the order parame-
ters and to order $(n/t)^2$ $(t''/t)^2$ this expression is the most ters and to order $(\eta/t)^2$, $(t''/t)^2$, this expression is the most
general one consistent with symmetry but for the quartic general one consistent with symmetry, but for the quartic terms, in the interest of simplicity, we have assumed that the SOC is weaker than the band mixing, and so have enforced spin rotational symmetry. Since $|v_i| \ll u$, the terms on the third line are not qualitatively important. When the action is derived from any form of BCS theory, it is possible to show that γ and $J_i > 0$. Thus, there are two possible phases depending on the sign and magnitude of a_1 : (a) For $a_1 > \text{Min}[0, a_2]$, there are time-reversal symmetry preserving ''B'' phase states (analogous to the B phase in ³He) in which $\hat{\Omega}_x \cdot \hat{\Omega}_y = \hat{\Omega}_x \cdot \hat{z} = \hat{\Omega}_y \cdot \hat{z} = 0$

FIG. 3 (color online). (a) In the absence of any band mixing, the triplet state within the xz orbital (red [light grey]) has k_x -wave symmetry and has line nodes near $k_y = \pi/2$ (dashed line). The condensate on the yz orbital (grey) is related to the one shown here by a 90-degree rotation. (b) The chiral state which results when small band mixing perturbations are taken into account. The relative phase factors on different portions of the Fermi surface are shown.

and $\theta_x = \theta_y$. Depending on the sign of a_2 , either $\hat{\Omega}_x = \hat{x}$ or $\hat{\Omega}_x = \hat{y}$. (b) For $a_1 > \text{Min}[0, a_2]$, there is a "chiral $p + ip'$ state (analogous to the A phase in He3) with $\hat{\Omega}_x$ = $\hat{\Omega}_y = \hat{z}$ and $\theta_x - \theta_y \pm \pi/2$. All other configurations have a higher Free energy.

The parameters a_i can be related to differences of susceptibilities of the noninteracting system, and so can be computed directly from the assumed band structure. For the stated parameters, we find that $a_1 <$ Min[0, a_2], so the chiral state is preferred. However, the balance is delicate, and this conclusion is not robust against small changes to the model.

Next, we address the fate of the gap nodes when $\delta H \neq$ 0. We have studied the Bogoliubov de Gennes (BdG) Hamiltonian for the chiral state using the gap functions derived in the previous section. Generically, the resulting state is nodeless. However, although the nodes are not topologically stable, they are parametrically small: where a gap node occurs for $\delta H = 0$, the induced gap is $\sim \Delta_0[{\cal O}(t^{1/2}/t^2)+{\cal O}(\eta^2/t^2)]$. The energy scale of these
van minima is therefore 2 orders of magnitude smaller gap minima is therefore 2 orders of magnitude smaller than the transition temperature.

Topological properties and edge currents.—Next, we consider the topological properties of the system assuming that a_1 < Min[0, a_2], so the chiral state is preferred. The BdG Hamiltonian for the quasiparticle excitations in the superconducting state can then be expressed in terms of Anderson pseudospins as

$$
H_{\text{BdG}} = \sum_{\nu,\vec{k}} \Psi^{\dagger}_{\nu\vec{k}} [\vec{\delta}_{\nu}(\vec{k}) \cdot \vec{\tau}] \Psi_{\nu\vec{k}}.
$$
 (11)

where $\Psi_{\nu \vec{k}}$ are Nambu spinors, $\nu = \alpha$, β runs over the two quasi-1D hands $\vec{\tau}$ are the Pauli matrices, and the pseudoquasi-1D bands, $\vec{\tau}$ are the Pauli matrices, and the pseudo-Zeeman field is

$$
\vec{\delta}_{\nu}(\vec{k}) = \{ \text{Re}[\Delta_{\nu}(\vec{k})], \text{Im}[\Delta_{\nu}(\vec{k})], \epsilon_{\nu}(\vec{k}) - \mu \}. \qquad (12)
$$

For the chiral p-wave state, the pseudospin has the form of a skyrmion in momentum space: it points along the

on the Fermi surface, it lies in plane, winding by 2π around $-\hat{z}(\hat{z}+\hat{z})$ -direction inside (outside) the Fermi surface, and the Fermi surface. The topological properties of the chiral state come from the integer skyrmion number

$$
\mathcal{N}_{\nu} = \frac{1}{4\pi |\vec{\delta}_{\nu}(\vec{k})|^3} \int d^2k \vec{\delta}_{\nu} \cdot (\partial_x \vec{\delta}_{\nu} \times \partial_y \vec{\delta}_{\nu}) \qquad (13)
$$

where $|\vec{\delta}_{\nu}(\vec{k})| = \sqrt{[\epsilon_{\nu}(\vec{k}) - \mu]^2 + |\Delta_{\nu}(\vec{k})|^2}$. The net num-
her of chiral quasiparticle modes at the edge of the superber of chiral quasiparticle modes at the edge of the superconductor is given by the Skyrmion number, and so long as $\mathcal{N}_{\nu} \neq 0$, these modes are topologically protected, and cannot be localized by backscattering.

As \mathcal{N}_{ν} is an integer, small changes in the spectrum do not affect it. However, it is odd under $\Delta_{\nu} \rightarrow \Delta_{\nu}^{*}$ (i.e., upon transforming $n + i n \rightarrow n - i n$) or under a particletransforming $p_x + ip_y \rightarrow p_x - ip_y$ or under a particle-
hole transformation $\epsilon = u \rightarrow u = \epsilon$. As can be seen hole transformation, $\epsilon_{\nu} - \mu \rightarrow \mu - \epsilon_{\nu}$. As can be seen
in Fig. 1, hybridization between the two quasi-1D bands in Fig. [1,](#page-1-0) hybridization between the two quasi-1D bands results in the closed α and β Fermi surfaces, the former electronlike and the latter holelike. Consequently, in a chiral $p_x + ip_y$ state, $\mathcal{N}_\alpha = -\mathcal{N}_\beta$, or in other words
the net skyrmion number is zero so (to the extent that the the net skyrmion number is zero so (to the extent that the xy band can be neglected) it is not a topological superconductor. The chiral edge modes along the boundary of the superconductor and along domain walls are not protected: in the presence of disorder or interactions that scatter a pair from one Fermi surface to the other, the counterpropagating edge modes from the two bands are localized [\[21\]](#page-3-18).

While disorder can quench the currents associated with the Majorana modes, there is still no symmetry principle which *prohibits* the existence of edge currents. Indeed, using simplified models with rotational invariance, previous researchers [\[8,](#page-3-6)[9](#page-3-7)] have inferred the existence of nonuniversal but substantial edge currents of bulk origin, which they relate to the orbital moment of a $p + ip$ condensate. To address this issue, we have considered the problem in the strong pairing limit, in which bosons (representing a p-wave pair) live on the lattice of Ru-Ru bonds, with pure imaginary hopping between nearest-neighbor bonds to insure a $p + i p$ character of the Bose condensed state. It is easy to see, by solving this problem in the presence of a boundary, that there are no edge currents in the Bose condensed state despite the absence of a symmetry forbidding them. Thus, the spontaneous currents at the boundary are finite on a lattice only in the BCS regime, in which quasiparticle edge modes are present. Since these edge modes are in turn localized in the quasi-1D superconductor, the associated electrical currents are vanishingly small. We conjecture that, more generally, lattice effects will greatly suppress any bulk contribution to the edge currents.

Discussion.—It follows from general arguments [\[23\]](#page-3-20) that near T_c , superconductivity can arise either in the $\{\alpha, \beta\}$ pockets or in the γ pocket; below T_c , superconductivity is induced in the subdominant Fermi surfaces via a tivity is induced in the subdominant Fermi surfaces via a proximity effect

$$
\delta H_{\text{prox}} = J' \sum_{\nu \neq \nu'} c_{i\nu\uparrow}^\dagger c_{i\nu\downarrow}^\dagger c_{i\nu'\downarrow} c_{i\nu'\uparrow}, \tag{14}
$$

with $J' \ll U$ [[23](#page-3-20)]. Because of the weakness of this proximity effect, it can be expected that for a range of temperatures $J'(\Delta/E_F) \ll T < T_c$, superconductivity is present es-
sentially only on the dominant portions of the Fermi sursentially only on the dominant portions of the Fermi surfaces. Nonetheless, in the present case, this coupling produces a small gap on the xy Fermi surface, which then adds to the skyrmion number; while the energy scales involved are likely too small to affect the results of any practical experiment, ultimately the proximity effect restores the topological character of the chiral superconducting state.

As we have shown, it is unavoidable, given the band structure of $Sr₂RuO₄$, and assuming the interactions are weak, that the superconductivity arises primarily on the quasi-1D bands. Within this framework, there is a natural explanation for the surprising absence of superconductivity in the closely related bilayer compound $Sr_3Ru_2O_7$; the bilayer splitting in $Sr_3Ru_2O_7$ primarily affects the quasi-1D bands, leaving the 2D d_{xy} band essentially unchanged.

Admittedly, we cannot rule out the possibility that strong coupling effects will change this conclusion. However, the absence of experimentally detectable edge currents is difficult to reconcile with a state which primarily involves the 2D bands. Further analysis concerning this issue will be postponed to a future paper [[21](#page-3-18)].

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