Quantum paramagnet in a π flux triangular lattice Hubbard model

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We propose the π flux triangular lattice Hubbard model (π-THM) as a prototypical setup to stabilize magnetically disordered quantum states of matter in the presence of charge fluctuations. The quantum paramagnetic domain of the π-THM which we identify for intermediate Hubbard U is framed by a Dirac semi-metal for weak coupling and by 120° Néel order for strong coupling. Generalizing the Klein duality from spin Hamiltonians to tight-binding models, the π-THM maps to a Hubbard model which corresponds to the \((J_H, J_K) = (-1, 2)\) Heisenberg-Kitaev model in its strong coupling limit. The π-THM provides a promising microscopic testing ground for exotic finite-U spin liquid ground states amenable to numerical investigation.

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Introduction. Two-dimensional quantum paramagnets such as spin liquids or valence bond crystals are quantum states of matter that, albeit their enormous diversity from a theoretical standpoint, are hard to find in experimental scenarios [1–4]. At the level of theoretical identification in microscopic models, recent numerical advances such as two-dimensional density matrix renormalization group [5–7], pseudofermion renormalization group [8], or variational Monte Carlo [9, 10] could provide substantiated support for spin liquid regimes. Predominantly, the strong coupling limit of a Mott state is considered which is parametrized by spin exchange interactions.

An exception constitutes the work by Meng et al. on the Hubbard model for the honeycomb lattice, where quantum Monte Carlo algorithms avoid the sign problem due to lattice bipartiteness [11]. Small system sizes suggested a non-magnetic insulating regime without valence bond crystal order [11]. As larger scale calculations [12] and more refined determinations of the order parameter [13, 14] revealed, however, the metal insulator transition turns out to be of Gross-Neveu type, where antiferromagnetic order sets in immediately. This is confirmed by cluster methods operating at intermediate Hubbard U [15, 16]. What can still be taken as a motivation from this finding is that a Dirac metal for weak coupling might contribute to a promising scenario for an unconventional metal-insulator transition and exotic phases at intermediate coupling, which is the starting point of our analysis.

In this Letter, we propose the Hubbard model on the π flux triangular lattice (π-THM) as a prototypical candidate for quantum paramagnetic phases at intermediate coupling. In its weak coupling limit, the band structure of the π-THM is semi-metallic, exhibiting the same low-energy behavior as graphene with a different Fermi velocity. The stability of this semi-metal with respect to weak local Coulomb interactions follows from generic properties of Dirac electrons [17, 18]. In its strong-coupling limit, positive and negative hoppings give rise to the same spin exchange amplitude \(J = 4(\pm t)^2/U\), rendering the π-THM to be identical to the nearest-neighbor Heisenberg model on the triangular lattice yielding 120° Néel order [19]. Generalizing the Klein duality [20–23] from spin models to tight-binding models, we can relate the π-THM to a transformed Hubbard model with bond-selective Kitaev-like hopping amplitudes. The strong coupling limit of this Klein-transformed model is given by the \((J_H, J_K) = (-1, 2)\) Heisenberg-Kitaev model.

As the weak and strong coupling limits are fixed, it remains to be investigated whether there is a direct semi-metal to magnet transition, or whether an intermediate paramagnetic domain emerges at the metal insulator transition. We will explicate below that perturbing away from its infinite-U limit, the short-range resonating valence bond (RVB) loops lower the energy in the π-THM more significantly than for the regular Hubbard model on the triangular lattice (THM). These perturbative arguments are supplemented by the calculation of single-particle spectral functions and ordering tendencies via variational cluster approximation (VCA). For intermediate Hubbard U, we find an extended non-magnetic insulating regime, which promises to host unconventional quantum paramagnetic states of matter.

π-THM. We consider a triangular lattice with an alternating flux pattern such that a triangle threaded by a π flux is surrounded by three triangles which are flux-free (Fig. 1a). (Note that triggered by the success in formulating and manufacturing flux lattices through artificial gauge fields in ultra-cold atomic gases [24–26], flux patterns in lattice models has become an experimentally relevant topic in contemporary AMO physics.) In Fig. 1a, the signs of the real nearest-neighbor hoppings \(t_{ij}\) are shown which reproduce this flux pattern; the two-atomic
the Dirac nodes yields the Lorentz-invariant Dirac theory. The Brillouin zone (black) is spanned by the reciprocal energy); the lower band follows from particle-hole symmetry. The unit cell is shown in yellow spanned by the primitive vectors \( \mathbf{b}_1 = \frac{2\pi}{\sqrt{3}}(1, \sqrt{3}) \) and \( \mathbf{b}_2 = \frac{2\pi}{\sqrt{3}}(-1/2, \sqrt{3}/2) \). (c) four-sublattice structure of a Klein transformation. The labels ‘\( \pi \)’, ‘\( \gamma \)’ and ‘\( \alpha \)’ indicate the axis around which a spin rotation of angle \( \pi \) is performed. Full dots are lattice sites where the spins remain unchanged.

The unit cell is shown in yellow spanned by the primitive vectors \( \mathbf{a}_1 = (\sqrt{3}/2, 1/2) \) and \( \mathbf{a}_2 = (-\sqrt{3}, 1) \). We set the lattice spacing \( a \equiv 1 \) throughout the paper. Note that the band structure is spin-degenerate and particle-hole symmetric. The Bloch matrix reads \( h(k) = \sum_{\sigma} d(k) \cdot \sigma \) where \( \sigma^\alpha \) corresponds to Pauli matrices related to the sublattice degree of freedom and

\[
d(k) = t \begin{pmatrix} 1 + \cos a_1 k + \cos a_2 k - \cos (a_1 + a_2) k & \sin a_1 k - \sin a_2 k + \sin (a_1 + a_2) k \\ \sin a_1 k - \sin a_2 k + \sin (a_1 + a_2) k & 2 \cos a_1 k \end{pmatrix}.
\]

We find the single particle spectrum \( \varepsilon^\pm_\alpha = \pm \sqrt{\varepsilon^2 + 4a^2} \) which is shown as a contour plot in Fig. 1b. The Dirac nodes are located at \( K^\pm = (\pm \pi/\sqrt{3}, 0) \). Expanding around the Dirac nodes yields the Loretz-invariant Dirac theory of graphene, along with valley and spin degeneracy and a bare Fermi-velocity \( v_F = \sqrt{6}t \). Note that this type of band structure has been previously mentioned as a mean field spectrum of a U(1) liquid candidate (dubbed U1B) [27]. Adding Hubbard interactions, we find the \( \pi \)-THM governed by the Hamiltonian

\[
H_{\text{THM}} = \sum_{(ij), \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} + U \sum_i n_{i\uparrow} n_{i\downarrow},
\]

where \( n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \) denotes the density operator of electrons at site \( i \) with spin \( \sigma \).

**Klein-duality map from a Kitaev-Hubbard model.** The \( \pi \) flux pattern on the triangular lattice allows to draw subtle connections to iridium-based transition metal oxides and Heisenberg-Kitaev models [21]. Originally proposed for the honeycomb iridates (Na,Li)\(_2\)IrO\(_3\) [21], the Heisenberg-Kitaev model reads

\[
H_{\text{HK}} = \sum_{(ij)} J_H S_i S_j + J_K S_i^z S_j^z,
\]

where, for the triangular lattice, we define \( \gamma = x \) for bonds along the \( a_1 \) direction, \( \gamma = y \) along the \( a_2 \) direction, and \( \gamma = z \) along the vertical bonds.

We define the class of Kitaev-Hubbard models as tight-binding band structures subject to local Hubbard \( U \) which, in the limit of infinite \( U \), map onto a Heisenberg-Kitaev model (3). As explicated below, we can formulate a Klein duality map from our \( \pi \)-THM to such a Kitaev-Hubbard model. In the past, Klein dualities have been successfully applied to spin Hamiltonians [20–23]. Here, we generalize the Klein duality to Hubbard models, i.e., to creation and annihilation operators of electrons. As for the spin models, we define four sublattices on the triangular lattice [Fig. 1(c)], and then rotate the spin of the creation/annihilation operators on the different sublattices: we rotate the first sublattice around the \( x \) axis by \( \pi \), the second around the \( y \) axis by \( \pi \), the third around the \( z \) axis by \( \pi \), and the fourth sublattice remains unchanged [Fig. 1(c)]. Such spin rotations are easily accomplished by virtue of Pauli matrices, \( U_\alpha = \exp(i\frac{\pi}{2} \sigma^\alpha) = i\sigma^\alpha \) and \( U^{\dagger} = -i\sigma^\alpha \) for rotations around the \( \alpha \) axis \( (\alpha = x, y, z) \). The Klein-transformed version of Eq. (2) is given by a Kitaev-Hubbard model with a kinetic term \( H_0 = i(\sum_{ij} \nu_{ij} c_{i\sigma}^\dagger \sigma^\alpha c_{j\beta}^\dagger \sigma^\beta) \) where \( \gamma = x, y, z \) are defined as in (3), and \( \sigma^\gamma \) denote Pauli matrices describing the spin degrees of freedom. The phase convention \( \nu_{ij} = \pm 1 \) is chosen such that hopping in \( a_1 \), \( a_2 \), and \( (2a_1 + a_2) \) directions is positive and in opposite directions negative. The Hubbard term \( U n_{i\uparrow} n_{i\downarrow} \) remains invariant under the Klein map. In the strong coupling limit this Kitaev-Hubbard model transforms into the \( (J_H, J_K) = (-1, 2) \) Kitaev-Heisenberg model of Eq. (3).

Depending on the specific values of \( J_H \) and \( J_K \), the model in Eq. (3) might give rise to nonmagnetic phases of triangular layered iridate compounds [28, 29]. From the classical analysis, the \( (J_H, J_K) = (-1, 2) \) point in Eq. (3) is surrounded by a \( \mathbb{Z}_2 \) vortex lattice [30]. As such, the Klein map suggests that charge fluctuations in the \( \pi \)-THM, as implied by finite \( U \), may trigger similarly interesting effects as for the vortex lattice.

**Variational Cluster Approximation.** VCA is a quantum cluster approach to compute single-particle spectral functions for interacting many-body systems [31]. In a
which are important for the analysis of the parameters which may also include the bare hopping amplitudes, the chemical potential as well as all single-particle correlations. Embedded into a grand-canonical ensemble, the problem, while the method still includes spatial quantum correlations (Figs. 3(b)-(d)), while the general trend from previous VCA investigations of the regular THM [33] derive from our consideration of cluster hopping variation.) This can be understood from a strong coupling expansion [34]. For the π-THM, up to order $t^4/U^3$, we find

$$H_{\pi-\text{THM}}^{(4)} = \left(4t^2/U + \frac{12t^4}{U^3}\right) \sum_{\langle ij \rangle} S_i S_j + \frac{12t^4}{U^3} \sum_{\langle\langle ij \rangle\rangle} S_i S_j + \frac{4t^4}{U^3} \sum_{\langle\langle\langle ij \rangle\rangle\rangle} S_i S_j - \frac{80t^4}{U^3} \sum_p \left[ (S_1 S_2)(S_3 S_4) + (S_2 S_3)(S_1 S_4) - (S_1 S_3)(S_2 S_4) \right].$$

where we use the standard notations $\langle ij \rangle$, $\langle\langle ij \rangle\rangle$, and $\langle\langle\langle ij \rangle\rangle\rangle$ for first, second, and third nearest neighbors, and $\sum_p$ indicates the summation over all parallelograms (including different orientations) which consist of two triangles, $\Delta$, where the long diagonal on the parallelogram is a link between the sites with indices “1” and “3”. Comparing the π-THM against the regular THM [35, 36], one notable difference is the reversed sign for the plaquette term coefficient in (4). We compute the strength of dimer resonances to investigate the effect of such higher order contributions. Given a dimer loop, the transition matrix element $|E_{12}|$ between two dimer configurations on that loop determines the energy gain associated with such a resonance. For a loop on a $2 \times 2$ plaquette, this reads

$$E_{12} = \langle 0 | H_{\pi-\text{THM}}^{(4)} | \sum \rangle,$$

where

$$|\sum\rangle = \frac{1}{2}(|\uparrow_1 \downarrow_2 \rangle - |\downarrow_1 \uparrow_2 \rangle)(|\uparrow_3 \downarrow_4 \rangle - |\downarrow_3 \uparrow_4 \rangle).$$

In Eq. 5 the Hamiltonian $H_{\pi-\text{THM}}^{(4)}$ is restricted to a $2 \times 2$ plaquette. Resonances for longer dimer loops may be calculated similarly. In Fig. 3, we show the energy gain $|E_{12}|$ for resonances on all dimer loops with a length of 4 and 6 lattice spacings. For the shortest 4-site loop (Fig. 3a), $|E_{12}|$ is larger for the π-THM than for the regular THM. This picture diversifies as we consider longer-loop contributions (Figs. 3(b)-(d)), while the general trend from the smallest loop size persists. The enhanced dimer resonances give a natural explanation for the quick drop of magnetic order in the π-THM upon decreasing $U/t$. 

Phase diagram. For the quantitative analysis, we employ a super-cluster construction with a 12-site and mirror-12-site cluster (see inset Fig. 2) We first pin the Dirac metal-insulator transition by determining the opening of the charge gap $\Delta_c$ at $U/t = 9.5$ (blue domain in Fig. 2). Note that this happens at comparably large $U$, in accordance with the small spectral weight of the Dirac metal nearby the Fermi level. In the infinite coupling limit, the nearest neighbor Heisenberg term $J = 4t^2/U$ dominates the virtual spatial fluctuation processes. We apply the Weiss field associated with $120^\circ$ Néel order and determine the response of the π-THM. We find magnetic order ranging only down to $U/t = 13.4$ (red domain in Fig. 2). This finding is remarkable, as the regular THM, investigated for the same setting, allows for magnetic ordering to the lower value of $U/t = 8.5$. (Quantitative deviations from previous VCA investigations of the regular THM derive from our consideration of cluster hopping variation.) This can be understood from a strong coupling expansion [34]. For the π-THM, up to order $t^4/U^3$, we find

$$H_{\pi-\text{THM}}^{(4)} = \left(4t^2/U + \frac{12t^4}{U^3}\right) \sum_{\langle ij \rangle} S_i S_j + \frac{12t^4}{U^3} \sum_{\langle\langle ij \rangle\rangle} S_i S_j + \frac{4t^4}{U^3} \sum_{\langle\langle\langle ij \rangle\rangle\rangle} S_i S_j - \frac{80t^4}{U^3} \sum_p \left[ (S_1 S_2)(S_3 S_4) + (S_2 S_3)(S_1 S_4) - (S_1 S_3)(S_2 S_4) \right].$$

where we use the standard notations $\langle ij \rangle$, $\langle\langle ij \rangle\rangle$, and $\langle\langle\langle ij \rangle\rangle\rangle$ for first, second, and third nearest neighbors, and $\sum_p$ indicates the summation over all parallelograms (including different orientations) which consist of two triangles, $\Delta$, where the long diagonal on the parallelogram is a link between the sites with indices “1” and “3”. Comparing the π-THM against the regular THM [35, 36], one notable difference is the reversed sign for the plaquette term coefficient in (4). We compute the strength of dimer resonances to investigate the effect of such higher order contributions. Given a dimer loop, the transition matrix element $|E_{12}|$ between two dimer configurations on that loop determines the energy gain associated with such a resonance. For a loop on a $2 \times 2$ plaquette, this reads

$$E_{12} = \langle 0 | H_{\pi-\text{THM}}^{(4)} | \sum \rangle,$$

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In Eq. 5 the Hamiltonian $H_{\pi-\text{THM}}^{(4)}$ is restricted to a $2 \times 2$ plaquette. Resonances for longer dimer loops may be calculated similarly. In Fig. 3, we show the energy gain $|E_{12}|$ for resonances on all dimer loops with a length of 4 and 6 lattice spacings. For the shortest 4-site loop (Fig. 3a), $|E_{12}|$ is larger for the π-THM than for the regular THM. This picture diversifies as we consider longer-loop contributions (Figs. 3(b)-(d)), while the general trend from the smallest loop size persists. The enhanced dimer resonances give a natural explanation for the quick drop of magnetic order in the π-THM upon decreasing $U/t$. 

FIG. 2. (Color online). Phase diagram of (2) as obtained by VCA. $U_{c1}$, $U_{c2}$, $\Delta_c$, and $m_{120^\circ}$ are calculated for a lattice covering with 12-site (mirror) clusters as sketched in the inset (the magnetization $m_{120^\circ} = 1$ denotes the saturation value). From single-particle spectra, there are three phases: semi-metal (SM), non-magnetic insulator (NMI), and $120^\circ$ Néel antiferromagnetic insulator (AFM).
Whether a valence bond crystal, i.e. the onset of translational symmetry breaking, or a spin liquid state might be preferred cannot be inferred from this consideration. (At least note that the dimer resonance does not significantly drop from a 2-site loop to 6-site loops, which might suggest a possibly sizable resonance to long-range dimer loops along the RVB liquid paradigm [37–39].) Similarly, our analysis does not allow to determine whether the non-magnetic insulating domain (Fig. 2) is composed out of one or several distinct paramagnetic phases.

Conclusion. We have proposed the Hubbard model on the $\pi$ flux triangular lattice to constitute a paradigmatic scenario for quantum paramagnets at intermediate coupling. Via VCA, we find a non-magnetic insulating regime for $9.5 < U/t < 13.4$ framed by a Dirac semi-metal and $120^\circ$ Néel order which only establishes itself close to the strong coupling limit because of significant quantum fluctuations. The dimer resonances of the $\pi$-THM provide further support for its propensity towards quantum paramagnetic phases.

Several directions might be interesting to follow up on this work. First, additional methodological approaches should be applied to further resolve the nature of the paramagnetic domain in the $\pi$-THM. Second, it is worth investigating possible experimental realizations in the context of ultra-cold atomic fermionic gases deposited in optical flux lattices. In addition, the Klein-transformed Hubbard model derived from the $\pi$-THM might be applicable to the iridate triangular compounds where a joint perspective from Heisenberg-Kitaev models and charge fluctuations due to finite Hubbard $U$ might be indispensable. Third, from a broader perspective, the Klein duality mapping of Hubbard models can establish a valuable new tool to derive interesting connections between different lattice Hamiltonians, where the one model allows to draw implications on the other.

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