

High-Temperature Phase Separation and Charge-Magnon Liquid in Kinetic Antiferromagnets

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Understanding mechanisms of quantum ordering in strongly correlated systems remains a central challenge in condensed matter physics, with implications for designing novel quantum materials. Here, we investigate kinetic antiferromagnetism on a triangular lattice under an applied magnetic field, where spin polarons emerge as charge-magnon bound states with mutual attraction. Using large-scale diagrammatic Monte Carlo simulations, we show that this interaction drives high-temperature phase separation into charge- and magnon-rich regions, bordered by polarized Mott insulating voids. Spectral function analysis reveals a substantial energy correction from magnon interactions, indicating that these carrier-rich regions form a strongly bound charge-magnon liquid. These findings shed new light on recent experiments on MoTe₂/WSe₂ moiré bilayers, underscoring kinetic magnetism as a unique pathway for strong intercarrier attraction and high-temperature quantum ordering, with potential applications in quantum materials.

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The doped Mott insulator, with charge carriers propagating on a spin-background, is a paradigmatic model of strongly correlated electronic systems that is central for identifying unconventional pairing mechanisms [1]. In this context, two fundamental energy scales arise: The kinetic energy results from delocalization of charge carriers, while the magnetic energy originates in super-exchange processes, which drive antiferromagnetism [2,3]. When the onsite repulsion greatly exceeds the bandwidth, superexchange interactions are suppressed, and the dynamics of the system effectively consists of carrier motion on a restricted subspace, described by the kinetic energy scale. In this scenario, magnetic order arises from delocalization: on a polarized background, interference between carrier paths is much stronger than with anticorrelated spins. If this interference is constructive, delocalization favors ferromagnetism; if it is destructive, it drives antiferromagnetism, as illustrated in Fig. 1.

Kinetic magnetism has historically attracted attention in the context of He₃ crystals [4,5]. However, the advent of transition metal dichalcogenide (TMD) moiré heterostructures has dramatically expanded the possibilities for experimental realization and control [6–9]. While delocalization generally promotes ferromagnetism on bipartite lattices [10,11], TMD moiré materials enable low-energy degrees

of freedom characteristic of a triangular lattice, supporting a wider range of behaviors, including antiferromagnetic interactions [12] and, in some cases, the ability to tune magnetic interactions *in situ* [13]. Related nonbipartite lattices may support kinetically driven resonating valence bond states [14].

A central theoretical prediction of kinetic antiferromagnetism is that, under an external field, charges and magnons

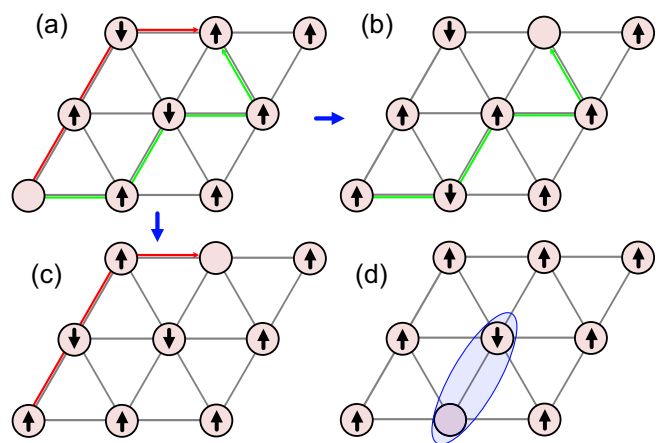


FIG. 1. Kinetic antiferromagnetism on the triangular lattice. In (a), the two paths lead to the same final position of the carrier. On a polarized background, these paths would interfere destructively, increasing the kinetic energy. However, in this initial configuration, the final states (b) and (c) are not identical, so no interference occurs. When destructive interference occurs, spin anti-correlation can reduce the kinetic energy, leading to antiferromagnetism. On a nearly fully polarized background, holes and magnons form strongly bound states, as shown in (d).

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form bound states, including bipolarons that may condense to form a superconducting state. The binding energy for a single charge and a single magnon is estimated to be $\epsilon_{cm} \approx 0.4227t$ in the strong coupling limit, suggesting that these spin polarons are potentially very stable [15]. At finite doping, the formation of a gas of such polarons is predicted to result in a magnetization plateau at low temperatures [16], accompanied by a pseudogap regime [17]. In the partially polarized regime, magnons may mediate attractive interactions between charge carriers, leading to the formation of bound states [15,16,18].

Experimental realization of spin polarons was recently reported in moiré bilayers [19]. For moderate hole doping, the magnetization curve flattens out in the polaronic regime. This effect is only seen at low temperature ($T/t \sim 0.027$) where spin fluctuations remain small. When particle-doping the same material, the magnetic susceptibility is instead enhanced due to the formation of ferromagnetic polarons [20]. With quantum gas microscopy, spin correlations in the proximity of carriers have been observed in both ferromagnetic and antiferromagnetic regimes [21–23].

The recent advances in kinetic antiferromagnetism suggest a mechanism for generating attractive interactions between charge carriers and producing novel magnetic properties. However, the efficacy of this mechanism remains unclear, and its implications for macroscopic systems are still an open question, as prior studies have primarily focused on zero-temperature scenarios with limited numbers of charge carriers.

In this Letter, we examine whether magnons can mediate significant attraction between charge carriers at finite temperatures, and, if so, explore the nature of the resulting phase and quantify the strength of these magnon-mediated interactions. By focusing on macroscopic systems with realistic thermal conditions, we aim to provide insights that bridge the gap between theoretical predictions and experimental realizations.

We tackle this problem using a minimalistic description of kinetic magnetism in the form of a triangular-lattice Hubbard model coupled to an external field

$$H = -\sum_{\sigma\langle ij\rangle} t c_{\sigma i}^\dagger c_{\sigma j} + \sum_i \left[U \hat{n}_{\downarrow i} \hat{n}_{\uparrow i} + \frac{B}{2} (\hat{n}_{\downarrow i} - \hat{n}_{\uparrow i}) - \mu \hat{n}_i \right] \quad (1)$$

in the strong-coupling limit $U/t \rightarrow \infty$. This scenario is relevant for existing moiré materials [7,8,24], including the experiment [19] where it is estimated that the energy scales of hopping and superexchange compare as $t/J \approx 20$.

We address the model (1) using diagrammatic Monte Carlo simulation, which is based on stochastic sampling of Feynman-type graphs [25–29]: The heart of this method is a random walk in the space of diagram topologies and their internal variables, based on the Metropolis algorithm. Diagrammatic elements are added, removed, or altered with

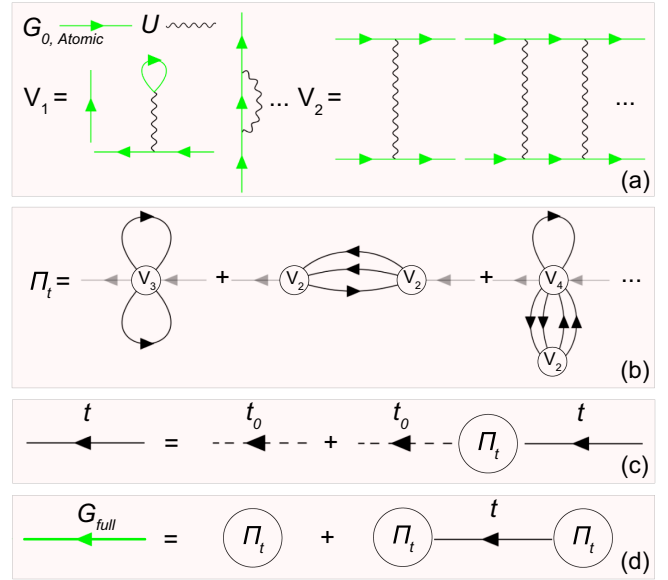


FIG. 2. Strong coupling diagrammatic Monte Carlo procedure. (a) The effective n -particle scattering vertices V_n are computed from the bare local Greens function and the contact interaction U . This computation is conducted in the atomic limit, and can be done exactly and nonperturbatively, even for $U \rightarrow \infty$. (b) The polarization operator of the hopping integral is obtained by from a diagrammatic expansion in V_N and the dressed hopping integral t . This is done stochastically with some max order in t . (c) The dressed hopping integral is obtained from the polarization operator via a Dyson/Bethe Salpiter type equation. The steps (b),(c) thus form a closed set of equations which are iterated until convergence. (d) The full Greens function is obtained from the polarization operator and the dressed hopping integral.

an acceptance ratio determined by the norm of a given diagram configuration. Via this random walk, a Monte Carlo integration is conducted for the self energy or a similar entity.

Diagrammatic Monte Carlo is an asymptotically exact method in the sense that the only systematic source of error is truncation of the series (which is generally necessary due to computational complexity). Furthermore, all results are obtained directly in the macroscopic limit, and for a convergent or resumable series, these can be obtained with known and typically small error bars. For a detailed introduction to diagrammatic Monte Carlo, see Ref. [25].

To access the strongly correlated regime, we use a variation known as strong-coupling diagrammatic Monte Carlo (SCDMC), which was specifically developed for strong contact interaction [30–34]. The protocol is based on integrating out contact interaction to produce scattering vertices that describe effective interactions between electrons. These vertices are then connected by the hopping integrals. By using the dressed hopping integral and expanding only in skeleton diagrams, we obtain a set of closed equations that provide a self-consistent solution as illustrated in Fig. 2. The exact procedure used is outlined in [32].

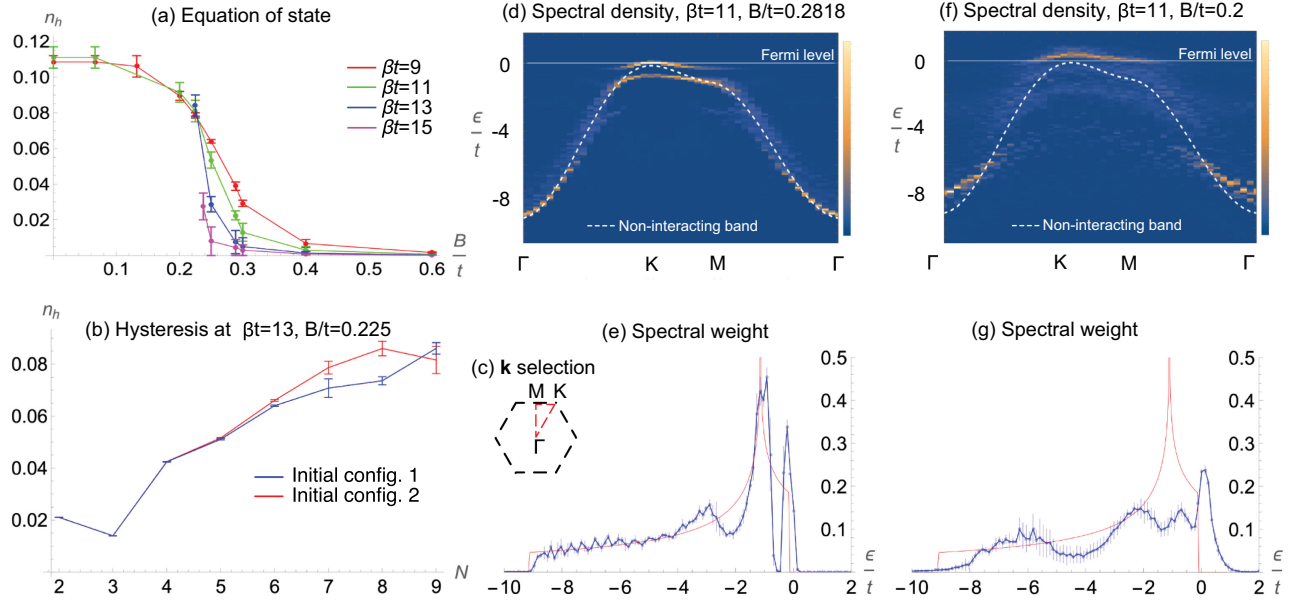


FIG. 3. Results obtained from strong coupling diagrammatic Monte Carlo. (a) Carrier density n_h as a function of the external magnetic field B with chemical potential $\mu/t = 3$ and inverse temperatures $\beta t = 9, 11, 13, 15$. Around $B/t \sim 0.25$ the carrier density declines rapidly with the magnetic field, revealing a large susceptibility which we interpret as resulting from phase separation into a carrier-rich charge-magnon liquid and a Mott insulator with few dopants. (b) Equation of state for $\beta t = 13$ and $B = 0.225t$ as a function of expansion order, obtained from two different initial configurations. At orders $N = 7, 8$ we observe that two solutions coexist, consistent with a phase separating system. (c) Illustrates the cut in momentum space used to plot spectral functions of the majority spin component. The spectra at $\beta t = 11$ and $B/t = 0.2818$ (d) reveals a “polaronic” subband of charges interacting with magnons. The corresponding spectral weight (e) indicates that this subband is gapped from the remaining spectral features. At $\beta t = 11$ and $B/t = 0.2$, the spectral function (f) becomes smeared, and the polaronic subband now overlaps with the rest of the spectrum (g). The spectral weight of fully polarized systems is shown in red (e),(g). The width of the polaronic subband in (d) is estimated to $w_p \sim 0.5t$, while it is notably broader in (f). Further discussion of the spectral function is given in Supplemental Material [36].

The principal observable produced in our simulations is the Gutzwiller-projected Greens function, defined on the permitted subspace [31],

$$\tilde{G}_\sigma(x-x') = \langle T[1-n_{-\sigma}(x')]c_\sigma^\dagger(x')c_\sigma(x)[1-n_{-\sigma}(x)] \rangle, \quad (2)$$

where x, x' refer to points in space-time. From the Greens function, we derive two key observables, the equation of state and the quasiparticle spectrum. The former is obtained from noting that the carrier density is given by $-\tilde{G}(\mathbf{r}=0, \tau \rightarrow 0^+)$. The latter, denoted by $A(\mathbf{k}, \epsilon)$, is related to the Greens function via

$$\tilde{G}(\mathbf{k}, \tau) = \int d\epsilon A(\mathbf{k}, \epsilon) \frac{e^{-\epsilon\tau}}{1 + e^{\beta\epsilon}}, \quad \tau < 0, \quad (3)$$

and can be obtained through simulated annealing [35]. The total density of states is then obtained from

$$d(\epsilon) = \int \frac{d\mathbf{k}}{(2\pi)^D} A(\mathbf{k}, \epsilon). \quad (4)$$

The energy is discretized so that ($\epsilon \rightarrow \epsilon_i; 1 \leq i \leq N_E$). We chose $N_E = 121$ as a compromise between accuracy and numerical stability.

The diagrammatic series must be truncated at some maximum order N , which is dictated by computational complexity. We are able to obtain solutions up to orders $N = 7-9$, depending on model parameters. Our estimates for the equation of state are based on a progression of calculations where we monitor how the answer changes with the expansion order. A complete record of this process is provided in Supplemental Material [36].

In a self-consistent expansion, multiple solutions can theoretically be obtained if the free-energy landscape exhibits multiple minima. For this reason, we solve the problem using multiple initial condition: Using the solutions from lower expansion orders as initial guesses for the dressed hopping integral implies starting at a lower carrier concentration. We complement this approach by also using initial conditions with a higher carrier concentration. In most of the parameter space, we only find a single solution, but in one case, we find hysteresis, as discussed below.

Figure 3 summarizes the results of the diagrammatic simulations. Panel (a) shows the equation of state as a function of the external field B . In the region $B/t \sim 0.25$, we observe a sharp drop in carrier density, which becomes more pronounced as the temperature decreases. At $\beta t = 13$,

most of the decline occurs within $B = 0.225\text{--}0.25t$, a range of just $0.025t$. At $\beta t = 15$, lower magnetic fields cannot be resolved due to convergence issues in the diagrammatic series, although the trend at stronger fields remains consistent. In the grand canonical ensemble, the presence of a large susceptibility, $\chi_{n,B} = \partial n / \partial B$, which increases at lower temperatures, is suggestive of phase separation.

To test the conjecture of phase separation, we use alternative initial configurations to identify signs of hysteresis. Figure 3(b) provides two series computed at $\beta t = 13$, $B/t = 0.225$. The blue curve is obtained by using a solution from the previous expansion order, as explained above. For the red curve, a solution obtained at a weaker field, and thus greater carrier density, was used for initial condition. At orders $N = 7, 8$ we observe that this leads to an alternative solution. At order $N = 9$, the first solution appears to become unstable, but this is most likely an artifact of numerical noise; see Supplemental Material for details [36].

The difference in carrier density between these solutions is small, indicating proximity to a bifurcation point where a second solution emerges. At this stage, the system separates into two phases with slightly different carrier densities. However, as shown in Fig. 3(a) the carrier density of the low-density phase drops sharply with decreasing temperature, suggesting that this phase evolves toward a nearly undoped Mott insulator as the system is cooled. At higher temperatures, we found that with alternative initial configurations, the systems converged to the same solution, but only very slowly, consistent with a flat free-energy landscape which would be expected close to a phase transition.

Figures 3(d)–3(g) show the spectral function and density of states at $\beta t = 11$ with $B/t = 0.2818$ (d), (e) and $B/t = 0.2$ (f), (g) computed at an expansion order $N = 7$, for the majority spin component. In the former case, the carrier density is small, at $n_h \sim 2\%$. The spectral density (d) reveals a polaronic subband that is separated from the remaining spectral features, consisting of carriers that reduce their kinetic energy by interacting with magnons in the environment. From the spectral weight (e) it is apparent that this subband is gapped from other degrees of freedom, consistent with the conjecture of a pseudogap phase in the polaronic metal [17]. It should be stressed that the gap is not situated at zero energy due to thermal spin and charge fluctuations. At zero temperature, we expect to see a gap at the Fermi level. The width of the polaronic subband can be estimated to $w_p \approx 0.5t$.

At a weaker field of $B/t = 0.2$, the carrier density increases to $n_h \sim 9\%$. The spectral function (f) now reveals a subband that is less well-defined, while remaining features are notably smeared. The density of states (g) shows that the polaronic subband is no longer gapped from the rest of the degrees of freedom. The width of the subband can for this reason not be completely made out,

but a conservative estimate gives that $w_p > t$ in this case, and there is a notable tail at positive energy.

The spectral function reveals two essential implications for understanding polaronic metals. First, the equation of state [Fig. 3(a)] shows that the carrier density drops sharply within a narrow magnetic field interval, $\delta B = 0.025t$. This corresponds to a polaron energy shift of $\delta\epsilon_p = \frac{3}{2}\delta B = 0.0375t$, which is more than an order of magnitude smaller than the width of the polaronic subband. Such a large magnetic susceptibility cannot be attributed to band flatness alone, providing strong evidence for phase separation.

Second, at higher carrier densities, the polaronic subband broadens markedly. Its high-energy tail extends to $\epsilon \approx t$, while the band top lies at $-0.1t$, implying a maximal carrier binding energy of $\epsilon_b \sim 1.1t$. This is substantially larger than the binding energy of an isolated polaron. The size of this correction indicates that polarons no longer behave as weakly interacting particles, but instead strongly hybridize.

We interpret this regime as a *charge-magnon liquid* (CML)—a quantum state where spin polarons have effectively “melted” and formed a dense, hybridized liquid. Crucially, the transition to this liquid phase can occur even at moderate total carrier densities due to strong interpolaron attraction and the emergence of phase-separated domains. In this sense, *phase separation serves as a mechanism that locally increases polaron density*, pushing the system into the hybridized regime despite globally low doping.

The charge-magnon liquid has several defining characteristics: spectral shift reflecting a reduction in carrier energy due to hybridization; spectral broadening of the charge sector, consistent with hybridization and strong interpolaron interaction; expected broadening of the magnon spectrum (not directly computed here, but anticipated); and phase separation at low average carrier densities, resulting from strong attraction.

The high onset temperature of phase separation ($T_c \sim t/13$) and the magnitude of the energy shift contrast sharply with behavior in doped Mott insulators on square lattices, where signs of carrier attraction remain weak at comparable temperatures [37].

This phase should leave observable signatures in the magnetic response. In a gas of isolated polarons, spin flips are associated with a discrete energy scale, leading to a magnetization plateau where the magnetic susceptibility vanishes [16], provided $\epsilon_{cm} \gg T$. Moreover, the magnetic response in such a regime should be nearly temperature independent.

In contrast, the CML phase exhibits magnons spanning a continuum of energies. This results in a finite magnetic susceptibility that displays a pronounced minimum—rather than a plateau—and varies significantly with temperature and doping. These features match experimental observations, where the susceptibility minimum becomes shallower with increasing carrier density [19], signalling the

breakdown of the isolated-polaron picture and the emergence of magnon-sharing among carriers.

A particularly informative experimental observable is the integrated magnetic response beyond the susceptibility minimum,

$$N_m = \int_{B_p}^{\infty} \chi_B dB, \quad (5)$$

where B_p denotes the field at which χ_B reaches its minimum or plateau. This quantity measures the number of magnons that remain in the system as the magnetization saturates. Experiments on $\text{MoTe}_2/\text{WSe}_2$ show that N_m increases significantly with doping [19], consistent with a scenario in which magnons are redistributed across the charge-magnon liquid and no longer confined to isolated polarons.

These observations collectively suggest that *polaron hybridization is not merely a theoretical possibility but plays an active role in the magnetic response of real materials*, even in the presence of long-range Coulomb repulsion.

In conclusion, we have investigated kinetic antiferromagnetism on a triangular lattice under an external magnetic field, focusing on magnon-mediated attraction between charge carriers. All the evidence point to the potency of this mechanism: the high-temperature onset of phase separation, the significant energy correction to carriers observed in the spectral function, and experimental indications of strong hybridization all underscore the potential of kinetic magnetism as a pathway to high-temperature quantum-ordered states, including pairing. This behavior contrasts sharply with Mott insulators on the square lattice and suggests that quantum gas spectroscopy [38–41] could reveal strong charge correlations, providing valuable insights into the nature of bound states. Additionally, our Letter highlights the need for ARPES experiments to estimate the energy scale of polaron hybridization in real-world materials with Coulomb interactions, offering critical experimental benchmarks for our predictions.

Twisted transition metal dichalcogenides (TTMDs) present an especially promising platform for further exploration of kinetic magnetism, as they allow for continuous, *in situ* tuning of correlations between ferromagnetic and antiferromagnetic regimes [13], enabling precise control over magnon-mediated attraction. At low carrier density, with reduced attraction, hybridization effects should be minimized, resulting in a gas of weakly interacting polarons and the emergence of a genuine magnetization plateau. Ultimately, these insights could inform the design of quantum materials with tunable magnetic and electronic properties, advancing the broader understanding of unconventional magnetic states in strongly correlated systems.

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Data availability—The data that support the findings of this article are openly available [42].

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