A quantum liquid with deconfined fractional excitations in three dimensions

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Excitations which carry “fractional” quantum numbers are known to exist in one dimension in polyacetylene, and in two dimensions, in the fractional quantum Hall effect. Fractional excitations have also been invoked to explain the breakdown of the conventional theory of metals in a wide range of three-dimensional materials. However the existence of fractional excitations in three dimensions remains highly controversial. In this Letter we report direct numerical evidence for the existence of an extended quantum liquid phase supporting fractional excitations in a concrete, three-dimensional microscopic model — the quantum dimer model on a diamond lattice. We demonstrate explicitly that the energy cost of separating fractional monomer excitations vanishes in this liquid phase, and that its energy spectrum matches that of the Coulomb phase in (3 + 1) dimensional quantum electrodynamics.

One of the great triumphs of twentieth-century physics was to show how the different physical properties of metals, magnets, semiconductors and superconductors could be understood in terms of the collective properties of a single elementary particle — the electron. For over fifty years, Landau’s concept of the Fermi liquid, a three-dimensional quantum liquid whose quasi-particle excitations carry the same spin and charge quantum numbers as an electron, has served as the “standard model” for metals. Recently, however, this theory has been challenged by experiments on a wide range of strongly-correlated materials, including quasi-one dimensional conductors, cuprate high-temperature superconductors and heavy Fermion systems near a quantum critical point [1,2].

These experiments prompt us to question whether new types of quantum liquid, capable of supporting new types of excitation might exist in nature? Indeed, excitations with fractional charge are known to exist in highly-doped, one-dimensional, trans-polyacetylene [3], and in the two-dimensional fractional quantum Hall effect [4]. However the existence of fractional excitations in three dimensions remains highly controversial. Indeed, since the understanding the quantum Hall effect is bound to the two-dimensional concept of “anyons” with fractional statistics [5], it has often been argued to be impossible.

An unambiguous way of resolving this question would be to find unbiased evidence of the existence a quantum liquid supporting deconfined fractional excitations in a concrete, three-dimensional microscopic model. This is the goal of this Letter. The model we consider is the quantum dimer model

\[
H = - \sum_{\langle \mathcal{O} \rangle} \left( |\mathcal{O}\rangle \langle \mathcal{O}| + \text{H.c.} \right) + \mu \sum_{\langle \mathcal{O} \rangle} \left( |\mathcal{O}\rangle \langle \mathcal{O}| + |\mathcal{O}\rangle \langle \mathcal{O}| \right). \tag{1}
\]

on a three-dimensional diamond lattice, where the first term describes the kinetic energy of hard-core dimers tunneling between different degenerate configurations on a hexagonal “flippable” plaquette, and \(\mu\) sets the ratio of potential to kinetic energy. This model was recently derived as an effective description of half-magnetization plateaux in Cr spinels [6, 7], and also describes spin-less fermions or hard-core bosons on a pyrochlore lattice at quarter filling, in the limit of strong nearest-neighbour interactions [20].

In fact quantum dimer models arise naturally as effective models of many different condensed matter systems, and provide a concrete realizations of several classes of lattice gauge theory [8, 9, 10, 11, 12]. As such, they have become central to the theoretical search for new quantum phases and excitations. A key feature of these models is the existence of a gapless “Rokhsar-Kivelson” (RK) point for \(\mu = 1\), at which all correlation functions exhibit algebraic decay [8]. Doping the model by removing a dimer introduces two monomers. Precisely at the RK point these monomer excitations are independent, deconfined excitations, each carrying half of the spin/mass/charge associated with a single dimer.

Field theory arguments suggest that, on bipartite lattices in three dimensions, the RK point “grows” into an extended

FIG. 1: (Color online) Conjectured form for the ground state phase diagram of the quantum dimer model on a bipartite lattice in 3D, as a function of the ratio \(\mu\) of potential to kinetic energy, following [6, 7, 12].
Here the potential energy dominates, and the ground state is eight-fold degenerate. To establish the validity of the proposed phase diagram Fig. 1, we need to connect this with the RK point $\mu = 1$, for which the ground state the equally weighted sum of all possible dimer configurations $R$. We accomplish this using a mixture of exact diagonalization, variational Monte Carlo (VMC) and Green’s function Monte Carlo (GFMC) techniques.

GFMC is a zero temperature quantum Monte Carlo technique which offers a systematic way of improving upon the variational wave function output by a variational Monte Carlo calculation. Where it converges, GFMC offers accuracy comparable with exact diagonalization. As an input for VMC, we use a trial wave function based on hexagon-hexagon correlations, with of order 40 variational parameters. Cluster sizes are limited by the rapid growth of the Hilbert space with system size — there are $1.3^N$ dimer coverings of an $N$-site diamond lattice cluster, and all of these contribute to the ground state wave function approaching the RK point. However we are able to access families of clusters with edges parallel to the [100], [110] and [111] directions which have the full (cubic) symmetry of the diamond lattice. Below we focus mainly on [100] clusters with $2L^3$ diamond lattice bonds, where $L = \{4, 6, 8, 10\}$.

In Fig. 3(a) we present numerical results for the order parameter $m_R$. This is defined as a sum of projections onto the $R$-state as a function of $\mu$, calculated using Green’s function Monte Carlo (GFMC) for [100] clusters with 128, 432, 1024 and 2000 bonds (lines and dots serve as a guide for the eye). Results are normalized such that $m_R = 1$ for $\mu \to -\infty$. Exact diagonalization (ED) results for 128 bonds are also shown. A sharp jump in $m_R$ can be seen for $\mu_c \approx 0.5-0.7$, suggesting a first order transition out of the $R$-state. (b) This coincides with a collapse in the string tension $\Delta_{1}/L$. The inset in panel (a) shows the finite-size scaling of $m_R$ at the RK point ($\mu = 1$). The inset in panel (b) shows the finite-size scaling of $\mu_c$. We obtain a value $\mu_c = 0.77 \pm 0.02$.
between GFMC and exact diagonalization results, and very close agreement between these and VMC. For larger systems there is a strong suggestion of a first order transition out of the R-state — a jump in \( m_R \) is observed for \( \mu_c \approx 0.7 \) in GFMC simulations (2000 bonds). We have studied the finite size scaling of \( \mu_c \) for series of [100], [110] and [111] clusters, and find \( \mu_c = 0.77 \pm 0.02 \) in the thermodynamic limit — see inset to Fig. 3(b) [23]. For the clusters considered, \( m_R \) still takes on a finite value for \( \mu > \mu_c \), but this is a finite-size effect. Exactly at the RK point \( m_R \) must vanish, and we can use our knowledge of the exact ground state to simulate much larger clusters. We find that that \( m_R \) scales to zero as \( L^{-3/2} \) (see the inset to Fig. 3a).

Another indicator of a crystalline, ordered phase is the linear, confining “string potential” associated with separating two fractional monomer excitations — illustrated in Fig. 2(b). Conversely, the energy cost of separating two fractional excitations by a distance \( L \) must vanish in the quantum liquid we are seeking. A suitable “string” configuration can be prepared by joining the ends of the string defect shown in Fig. 2(b) such that it connects opposite faces of a (periodic) cluster of linear dimension \( L \). Since GFMC preserves quantum numbers, it can be used to calculate the energy of the quantum eigenstate corresponding to such a classical string configuration, and the “string tension” calculated as \( \Delta_1/L \), where \( \Delta_1 \) is the energy of the string excitation relative to the ground state.

Deep inside the ordered state, \( \Delta_1 \) scales as \( \propto \mu L \), however the string tension \( \Delta_1/L \) collapses abruptly at the value of \( \mu \) for which the order parameter jumps — see main panel, Fig. 3(b). Taken together, these facts are strongly suggestive of a first order transition from a crystalline to a liquid phase with deconfined monomer excitations. But they do not yet prove the existence of the \( U(1) \) liquid we are looking for. In order to accomplish this, we must test explicitly the predictions of the relevant effective field theory.

The defining property of a dimer model is that every lattice site is touched by exactly one dimer. On a bipartite lattice, we can implement this constraint by associating a magnetic field \( B = \nabla \times A \) with each dimer and each empty bond. This field points from site to site along each bond such that \( \nabla \cdot B = 0 \) at every diamond lattice site [13, 14]. The total flux \( \phi = \int dS \cdot B \) through any plane (cutting bonds) in the lattice is a conserved quantity. Therefore, for periodic boundary conditions, the flux through a set of orthogonal planes defines a set of (integer) topological quantum numbers \( (\phi_1, \phi_2, \phi_3) \).

We choose to work in a gauge where \( \nabla \cdot A = 0 \) and in this Letter consider only flux sectors of the type \( (\phi, 0, 0) \), where \( \phi = 1 \) denotes the smallest finite flux and corresponds to the state with a single string defect described above.

This representation clearly has a lot in common with conventional electromagnetism and, following [14], we can use this analogy to write down a plausible long-wavelength action for the QDM on a diamond lattice

\[
S = \int d^3x dt \left[ \mathbf{E}^2 - \rho_2 \mathbf{B}^2 - \rho_4 (\nabla \times \mathbf{B})^2 \right],
\]

where \( \mathbf{E} = \partial_t \mathbf{A} - \nabla A_0 \) and \( \rho_4 > 0 \). We have studied \( \rho_2 \) in a perturbation theory about the RK point and find that it varies as \( \rho_2 \sim 0.6(0) \times (1 - \mu) \). For \( \mu > 1 \), the coefficient \( \rho_2 < 0 \), and the system chooses those dimer configurations with the maximum possible flux \( \phi \) — a set of isolated states which are not connected by any matrix element of the Hamiltonian Eq. (1). All excitations are then gapped. At the RK point \( \rho_2 \) vanishes, and all flux sectors contribute equally to the ground state. The system possesses gapless, transverse excitations with dispersion \( \omega = \rho_4 k^2 \). However for \( \mu \lesssim 1 \), \( \rho_2 > 0 \) and the analogy with electromagnetism is complete — transverse excitations are now “photons” with dispersion \( \omega = \sqrt{\rho_2} |k| [24] \).

These photons are the signature feature of the proposed \( U(1) \) liquid state, and offer a beautiful realization of Maxwell’s laws in a condensed matter system. However, Eq. (2) also contains information about the finite size scaling of the ground state energy, as a function of flux \( \phi \). A flux \( \phi \) through a cluster of volume \( L^3 \) corresponds to an average magnetic field \( B = \phi/L^2 \). In the \( U(1) \) liquid state, this magnetic field is uniformly distributed on the “coarse-grained” scale of the effective action Eq. (2). It then follows from Eq. (3) that the energy difference \( \Delta_\phi = E_\phi - E_0 \) between the ground state of the zero flux sector, and the lowest energy state of the sector with flux \( \phi \) scales as

\[
\Delta_\phi = E_\phi - E_0 = \rho_4 \phi^2 / L^2.
\]

Furthermore, by cycling dimers across the boundaries of the cluster, we can systematically construct the different flux sectors \( \phi \). This is the natural generalization of the “thought experiment” measuring the string tension \( \Delta_1/L \), above. Combining these results, we have a systematic means of studying the spectroscopic signatures of the proposed \( U(1) \) liquid state in simulations of a finite size systems.

In Fig. 4 we present this analysis for GFMC simulations of an \( L = 8 \) cluster of 1024 bonds. Deep within the ordered phase \( \Delta_\phi \propto L \times \phi \), and a plot of \( \Delta_\phi/\phi^2 \) at fixed \( L \) should therefore show a clear distinction between a \( U(1) \) liquid (\( \Delta_\phi/\phi^2 \propto \text{const.} \)), and an ordered phase (\( \Delta_\phi/\phi^2 \propto 1/\phi \)). For this cluster size a clear division is observed between \( \mu \geq 0.7 \) (liquid) and \( \mu \leq 0.6 \) (ordered). This is unambiguous evidence of a phase transition from a linearly confining phase into a \( U(1) \) liquid. The abrupt, qualitative change in the spectra indicates that this phase transition is first-order in character. Since we already know the nature of the confining phase — the R-state — this completes the phase diagram.

It is interesting to compare these results with recent work on the problem of strongly interacting, hard core bosons at half-filling on a pyrochlore lattice [17]. For large values of nearest-neighbour interaction, this hard-core bosonic model can be approximated by an effective quantum-loop model on the diamond lattice, closely related to the quantum dimer model studied here. Equal-time and static density correlation functions for the Bosonic model were calculated using a path integral quantum Monte Carlo approach, and an insulating “liquid”
state was found, whose finite-temperature correlations were well described by the predictions of a $U(1)$ gauge theory. However the excitations of this model have yet to be studied.

In conclusion, the numerical results presented in this Letter establish the existence of a $U(1)$ liquid ground state in the quantum dimer model on a diamond lattice for a finite range of parameters $0.7(7) < \mu < 1$, confirming the field theoretical scenario proposed by [8, 13, 14]. This liquid state has been demonstrated explicitly to support deconfined monomer excitations. These results therefore confirm the existence of fractional excitations in three dimensions.

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[20] In this special case, the Fermi sign can be “gauged” out of the problem by a suitable choice of convention for labeling lattice sites.
[21] For classical analogues to this problem, see e.g. C. Castelnovo et al., Nature 451, 42, (2008); G. Misguich et al. Phys. Rev. B 78, 100402(R) (2008)
[22] We have checked our GFMC results explicitly against exact diagonalization for small system sizes, and for large systems sizes against an expansion in $1/|\mu|$ for $\mu \to -\infty$, and perturbation theory in $1 - \mu$ for $\mu \to 1$. We find complete agreement in all cases. This (lengthly) analysis will be presented elsewhere.
[23] The $L^{-4}$-scaling follows from the fact that the $R$-state is gapped, while the competing liquid phase has linearly dispersing photon excitations.
[24] We work in units such that the volume of the 16-bond cubic unit cell is equal to 8. This, together with the normalization chosen for the the flux $\phi$, defines the units of $\rho_2$ and therefore the speed of light for photon excitations.