

Instantons and Massless Fermions in (2 + 1)-Dimensional Lattice QED and Antiferromagnets

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Lattice U(1) instantons in 2+1 dimensions have no fermion zero modes and do not break U(2n) flavor symmetry. Nevertheless, instantons in the presence of massless fermions interact via logarithmic potentials. These results are applied to the "flux" phase of a SU(n) antiferromagnet and the possibility of a transition from a gapless spin-liquid state to Néel order as n decreases from 4 to 2 is discussed.

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Quantum antiferromagnets can be described by compact U(1) gauge theories with matter fields. Since two-dimensional antiferromagnetism underlies high-temperature superconductivity, it is important to understand how different (2+1)-dimensional U(1) gauge theories behave. Both antiferromagnets and U(1) gauge theories can be studied systematically via $1/n$ expansions. Using this technique, Read and Sachdev recently demonstrated¹ that the Berry's phase of instantons (topological defects that are permitted because the gauge group is compact) leads to valence-bond order in one particular two-dimensional SU(n) antiferromagnet with massive charged bosonic matter fields, in accordance with a prediction by Haldane.² In contrast, the "flux" phase of a *different* two-dimensional SU(n) antiferromagnet contains massless relativistic fermions (the gap for fermionic excitations vanishes at discrete points in the Brillouin zone).³ In this Letter, I study instantons in the presence of massless fermions and conclude that instantons have no zero modes. Furthermore, the instantons interact via logarithmic potentials. I conclude by discussing the possibility that the Néel order known to occur in the physical SU(2) antiferromagnet corresponds to the dynamical formation of a fermion mass gap.

Instantons play a crucial role in (2+1)-dimensional compact pure U(1) gauge theory.⁴ In particular, the photon acquires a mass and static charges are confined when instantons are included. However, massless fermions can neutralize these effects. In one scenario, the instantons acquire fermion zero modes that spoil the mass generation mechanism.⁵ The SU(2) gauge group in that model spontaneously broke via the Higgs mechanism to (necessarily) compact U(1) and zero modes occurred because of topologically nontrivial long-range order in the Higgs field. (An index theorem for Dirac operators in odd-dimensional spaces⁶ can be applied when Higgs fields accompany the instanton. It was used in Ref. 5 to prove the existence of zero modes.)

The compact U(1) gauge group also arises naturally on the lattice. No Higgs fields are needed; instead, the lattice spacing a provides the necessary cutoff to make the instanton action ultraviolet finite. To investigate whether zero modes still exist, I solve the problem of

continuum massless fermions in the field of a single-point instanton. (I will show later that the wave functions are insensitive to lattice effects.) First, consider the problem of free fermions in spherical coordinates. The (imaginary-time) Lagrangian density is $\mathcal{L} = \bar{\psi}^{\alpha} \not{p} \psi_{\alpha}$, with $\alpha = 1, \dots, 2n$. (I consider only the case of an even number of fermion flavors; species doubling on the lattice allows me to ignore the case of an odd number.) Here $\not{p} \equiv \sigma \cdot \mathbf{p}$, $\bar{\psi} \equiv \psi^{\dagger} \sigma_3$, and the Pauli matrices obey the Clifford algebra $\{\sigma_{\alpha}, \sigma_{\beta}\} = \delta_{\alpha\beta}$. The Dirac operator \not{p} can be regarded as a Hamiltonian in three Euclidean dimensions. Following Besson⁷ I solve for the eigenmodes by using the identity $(\sigma \cdot \hat{\mathbf{r}})^2 = 1$. (Besson actually considered the problem of four-component fermions in four dimensions. The two-component fermions in three dimensions behave rather differently. One could assemble two two-component fermions into a single four-component spinor, but then the 4×4 representation of the γ matrices would contain *two* γ matrices, γ_4 and γ_5 , that anticommute with the Hamiltonian.) Thus

$$\begin{aligned} \not{p} &= (\sigma \cdot \hat{\mathbf{r}})^2 (\sigma \cdot \mathbf{p}) \\ &= (\sigma \cdot \hat{\mathbf{r}}) [\hat{\mathbf{r}} \cdot \mathbf{p} + i \sigma \cdot (\hat{\mathbf{r}} \times \mathbf{p})] \\ &= -i (\sigma \cdot \hat{\mathbf{r}}) [\partial / \partial r - (\sigma \cdot \mathbf{l}) / r]. \end{aligned}$$

Here \mathbf{l} is the orbital angular momentum. It does not commute with \not{p} but the total angular momentum $\mathbf{j} \equiv \mathbf{l} + \frac{1}{2} \boldsymbol{\sigma}$ does commute since $[\mathbf{j}, \sigma \cdot \hat{\mathbf{r}}] = [\mathbf{j}, \sigma \cdot \mathbf{l}] = 0$. Therefore, any eigenmode of \not{p} can be written as an eigenstate of \mathbf{j}^2 and $m \equiv j_z$. In particular, one of the two lowest partial waves ($j = \frac{1}{2}$, $m = \frac{1}{2}$) can be written as

$$\psi(r, \theta, \phi) = B(r) |\uparrow\rangle + A(r) (\sigma \cdot \hat{\mathbf{r}}) |\uparrow\rangle.$$

The $l=0$ radial wave function $B(r)$ and the $l=1$ wave function $A(r)$ satisfy the following coupled differential equations:

$$dB(r)/dr = iEA(r)$$

and

$$(d/dr + 2/r)A(r) = iEB(r).$$

These equations are solved with spherical Bessel functions of the first kind: $B(r) = j_0(kr)$, $A(r) = \pm i j_1(kr)$

with $E = \pm k$ [regularity at the origin forbids spherical Bessel functions of the second kind, $y_0(kr)$ and $y_1(kr)$, from appearing]. Note that the wave function does not vanish at the origin—it is the analog of the s -wave solution of the free Schrödinger equation.

The boundary conditions on the wave functions are determined by requiring the Dirac operator to be Hermitian. For any two wave functions ϕ and ψ we must have

$$\int d^3x \psi^\dagger \sigma \cdot \nabla \phi = - \int d^3x (\phi^\dagger \sigma \cdot \nabla \psi)^* .$$

Partial integration then implies that the following surface integral vanishes:

$$\int dS \cdot \psi^\dagger \sigma \phi = 0 .$$

For the particular case of $\phi = \psi$, this equation means that no net current flows across the boundary so probability is conserved. For $j = \frac{1}{2}$ waves inside a spherical box of radius R , the boundary condition requires either $j_0(kR) = 0$ or $j_1(kR) = 0$; therefore the radial momentum k is quantized.

We turn now to the problem of massless fermions interacting with a single instanton placed at the origin. Instead of a Dirac string, I follow Wu and Yang⁸ and define the vector potential locally by $A_r = A_\theta = 0$ and

$$A_\phi = \begin{cases} -\frac{g}{r \sin \theta} (\cos \theta - 1), & \mathbf{r} \in R_a, \\ -\frac{g}{r \sin \theta} (\cos \theta + 1), & \mathbf{r} \in R_b. \end{cases}$$

(Note that this choice of gauge obeys $\nabla \cdot \mathbf{A} = 0$.) The two overlapping regions R_a and R_b are defined by $R_a: 0 \leq \theta \leq \pi/2 + \delta$ and $R_b: \pi/2 - \delta \leq \theta \leq \pi$, where $0 < \delta < \pi/2$. The \mathbf{B} field points radially outward with strength g/r^2 and the wave functions defined separately in R_a and R_b are related by a gauge transformation in the region of overlap. The Hamiltonian is now given by \mathcal{P} , where $\mathbf{P} = \mathbf{p} - e\mathbf{A}$. To solve for the eigenmodes, I proceed similarly to the free case. Thus

$$\begin{aligned} \mathcal{P} &= (\sigma \cdot \hat{\mathbf{r}}) [\hat{\mathbf{r}} \cdot \mathbf{P} + i \sigma \cdot (\hat{\mathbf{r}} \times \mathbf{P})] \\ &= -i (\sigma \cdot \hat{\mathbf{r}}) \left[\frac{\partial}{\partial r} - \frac{\sigma \cdot \mathbf{L}}{r} - q \frac{\sigma \cdot \hat{\mathbf{r}}}{r} \right]. \end{aligned}$$

Here $q \equiv eg$ is integer or half-integer (to satisfy Dirac's quantization condition) and I have introduced the operator $\mathbf{L} \equiv \mathbf{r} \times \mathbf{P} - q\hat{\mathbf{r}}$. This operator obeys the angular momentum algebra $[L_a, L_b] = i\epsilon_{abc}L_c$. However, the "angular momenta" now have a minimum value of $|q|$ [note that $\mathbf{L}^2 = (\mathbf{r} \times \mathbf{P})^2 + q^2 \geq q^2$] and can be either integer or half-integer:⁸ $L = |q|, |q| + 1, \dots$. The analog of the total angular momentum \mathbf{j} is now $\mathbf{J} = \mathbf{L} + \frac{1}{2}\sigma$ which also commutes with $\sigma \cdot \hat{\mathbf{r}}$. The eigenstates of the Hamiltonian can be classified according to the eigenvalues of \mathbf{J}^2 and M . Now $J = |q| - \frac{1}{2}, |q| + \frac{1}{2}, \dots$ is not necessarily half-integer, reflecting the influence of the instanton.

Since all of the terms in the Hamiltonian scale as $1/r$, no bound states are possible. This observation was first made by Dirac⁹ in 1933 for the case of a nonrelativistic charged particle in the presence of a magnetic monopole. For any state $\psi_M^j(r, \theta, \phi)$ with energy $E = c$, there exists another state of energy $E = ck$ given by $\psi_M^j(kr, \theta, \phi)$. Thus, a continuum of states exists with no gap. Note that this argument no longer applies when Higgs fields are present since they supply an additional length scale that invalidates the above scaling argument. The lattice does provide a short length scale, but does not affect the wave functions qualitatively (see below).

The J^2, M eigenstates can be found using the "monopole harmonics" $Y_{q,L,M}$ of Ref. 8. In the notation of Ref. 7, these states are

$$\psi_M^j(r, \theta, \phi) = A_J(r) \mathcal{Y}_{M,L_+}^j(\theta, \phi) + B_J(r) \mathcal{Y}_{M,L_-}^j(\theta, \phi) .$$

Here $L_\pm \equiv J \pm \frac{1}{2}$,

$$\begin{aligned} \mathcal{Y}_{M,L_+}^j &\equiv \left[\frac{J+M+1}{2J+2} \right]^{1/2} Y_{q,L_+,M+1/2} | \downarrow \rangle \\ &\quad - \left[\frac{J-M+1}{2J+2} \right]^{1/2} Y_{q,L_+,M-1/2} | \uparrow \rangle \end{aligned}$$

and

$$\begin{aligned} \mathcal{Y}_{M,L_-}^j &\equiv \left[\frac{J-M}{2J} \right]^{1/2} Y_{q,L_-,M+1/2} | \downarrow \rangle \\ &\quad + \left[\frac{J+M}{2J} \right]^{1/2} Y_{q,L_-,M-1/2} | \uparrow \rangle . \end{aligned}$$

How does $\sigma \cdot \hat{\mathbf{r}}$ act on the \mathcal{Y}_{M,L_\pm}^j ? Since it commutes with \mathbf{J} , it can only mix the L_\pm states:

$$(\sigma \cdot \hat{\mathbf{r}}) \mathcal{Y}_{M,L_\pm}^j = a_\pm \mathcal{Y}_{M,L_+}^j + b_\pm \mathcal{Y}_{M,L_-}^j ,$$

where $a_+ = -b_- = 2q/(2J+1)$, $a_- = b_+ = -2K^{1/2}/(2J+1)$, and $K \equiv (J + \frac{1}{2})^2 - q^2$.

Consider first the lowest $J = |q| - \frac{1}{2}$ partial waves. Only the $L_+ = |q|$ wave function can appear in the lowest waves, since $L_- = |q| - 1$ is not an allowed eigenvalue. Thus, $B_J(kr) = 0$. In particular, for an instanton with the lowest possible charge ($|q| = \frac{1}{2}$) the $J=0$ wave function is $\psi_0^0 = A_0(kr) \mathcal{Y}_{0,1/2}^0$, where

$$\mathcal{Y}_{0,1/2}^0 = -\cos(\theta/2) | \uparrow \rangle - e^{i\phi} \sin(\theta/2) | \downarrow \rangle .$$

The radial function satisfies the following first-order differential equation:

$$-i(d/dr + 1/r)A_0(r) = \text{sgn}(q)EA_0(r) .$$

The solution to this equation is $A_0(r) = e^{ikr}/r$ with $E = \text{sgn}(q)k$. (The singularity in the wave function at $r \rightarrow 0$ is permitted now since the instanton field diverges as $r \rightarrow 0$.) Note that the energy of the incoming waves differs in sign from that of the outgoing ones. This behavior respects time-reversal (T) symmetry in the Ham-

iltonian picture, since both q and the fermion momentum change sign under T .

The boundary condition requires $|A_0(R)|^2=0$. Since the radial wave function has no zeros, it is forbidden. Indeed, standing $J=0$ waves do not exist because incoming and outgoing waves cannot be superposed since they have opposite energies. Furthermore, an additional boundary condition must be imposed at the origin (due to the singular nature of the wave function). Thus, $|A_0(0)|^2=0$ and again the $J=0$ wave function is forbidden. For instantons with larger charges the boundary conditions eliminate the lowest $J=|q|-\frac{1}{2}$ partial waves.

The higher partial waves ($J \geq |q| + \frac{1}{2}$) do not suffer from this defect since now $B_J(r) \neq 0$. The radial wave functions obey the following coupled differential equations:

$$\frac{dA_J}{dr} + \left(J + \frac{3}{2} - \frac{2q^2}{2J+1} \right) \frac{A_J}{r} + \left(\frac{2qK^{1/2}}{2J+1} \right) \frac{B_J}{r} = iE \frac{2qA_J - 2K^{1/2}B_J}{2J+1}$$

and

$$\frac{dB_J}{dr} - \left(J - \frac{1}{2} - \frac{2q^2}{2J+1} \right) \frac{B_J}{r} + \left(\frac{2qK^{1/2}}{2J+1} \right) \frac{A_J}{r} = -iE \frac{2K^{1/2}A_J + 2qB_J}{2J+1}$$

These equations are solved with higher spherical Bessel functions (see Ref. 7); like the free case, all the higher waves vanish at the origin. (Again spherical Bessel functions of the second kind are forbidden. Also, the boundary condition at the origin eliminates them.) Therefore, the wave functions are insensitive to the underlying lattice and should be accurate for $ka \ll 1$.

Note that the lattice could have severely modified one of the lowest partial waves and turned it into a zero mode, but the boundary condition at large R (where the continuum approximation should be good) eliminated it. Evidently, there are no normalizable zero modes since all the remaining partial waves vanish in the limit $r \rightarrow 0$. In fact, a direct numerical evaluation of the fermion wave functions on the lattice confirms this conclusion.¹⁰ This result also appears to hold for instantons with nonspherical symmetry.

The fermion contribution to the effective action can be computed for gauge configurations with no normalizable zero modes. For the case of a constant background field B^a in continuum QED, the massless fermions can be integrated out exactly;¹¹ the result is

$$\mathcal{L}_{\text{eff}} = \frac{n}{\pi^2} \zeta\left(\frac{3}{2}\right) \left[\left(\frac{e^2}{8} \right) F_{\mu\nu} F^{\mu\nu} \right]^{3/4}$$

Here $\zeta(x)$ is the Riemann ζ function [$\zeta(\frac{3}{2}) \approx 2.612$]

and $F_{\mu\nu} = \epsilon_{\mu\nu\alpha} B^\alpha$. The nonanalytic form of the effective action reflects the infrared divergences due to the massless fermions. It also follows from dimensional analysis [note that the combination eA_μ has the dimension (length)⁻¹ and there are no other length scales in the theory]. For nonconstant fields, additional terms such as $n(e^2 \partial_\sigma F^{\sigma\mu} \partial^\nu F_{\nu\mu})^{1/2}$ and $n(e^4 \partial_\sigma F^{\sigma\mu} \partial^\nu F_{\nu\mu} F^{\alpha\beta} F_{\alpha\beta})^{3/10}$ are possible.

Although lattice QED contains the length scale a , its long-wavelength behavior is the same as the continuum version. For example, a numerical calculation of the free energy of massless relativistic fermions on a spatial lattice and in a constant magnetic field shows the expected $|B|^{3/2}$ dependence in the small-field limit ($|eB|a^2 \ll 1$). (This system is just the Hofstadter problem for magnetic fluxes near π per plaquette.)

The fermion spectrum in the presence of a single instanton contains no zero modes so the action density for an instanton can be computed. In fact, the long-wavelength part can be determined up to an overall multiplicative constant: since $\mathbf{B} = g\hat{\mathbf{r}}/r^2$, all the terms in the effective action density have the form n/r^3 and clearly $\mathcal{L}_{\text{eff}} \propto n/r^3$. (Note that this simple inverse-power form does *not* occur for other gauge configurations.) Thus, a single instanton will have an infrared logarithmically divergent action. This divergence was noticed in a calculation of the two-point contribution to the effective action.¹² A direct calculation of the instanton action involves summing the logarithms of the zeros of the fermion Bessel functions; the preliminary result¹³ for the long-range part of the effective action is $S_{\text{eff}} = n\Gamma_q \times \ln(R/a)$, where $\Gamma_q \equiv 2(2|q|^{3/3} + q^2 + |q|)$.

The infrared divergence implies that two instantons of charge $\pm q$ at positions \mathbf{r}_a and \mathbf{r}_b interact via the (bare) potential $V(\mathbf{r}_a, \mathbf{r}_b) = 2n\Gamma_q \ln(|\mathbf{r}_a - \mathbf{r}_b|/a)$ instead of the $|\mathbf{r}_a - \mathbf{r}_b|^{-1}$ potential that occurs when dynamical matter fields are massive. In the absence of screening by dipole pairs, a Kosterlitz-Thouless transition into a confined phase would occur when n satisfies $2n\Gamma_{1/2} > 3$.¹² However, screening in dimensions $d \geq 3$ apparently weakens the logarithmic interaction to an inverse power-law form¹⁴ and the instantons are probably deconfined at all values of n .

$U(2n)$ flavor symmetry breaks to $U(n) \otimes U(n)$ if the fermions acquire a parity-conserving dynamical mass term.¹⁵ Parity-nonconserving mass terms are also possible, but a parity-conserving one seems to be energetically preferable.¹⁶ A single instanton does not induce such a term, since the fermion spectrum remains gapless in its presence. However, fermion masses can be generated *dynamically*. Pisarski¹⁷ used a $1/n$ expansion and Schwinger-Dyson equations for the fermion self-energy to conclude that symmetry breaking in noncompact QED occurs at all values of n . (The $1/n$ expansion is necessary to systematically control infrared divergences.) More refined calculations of the same type¹⁸ suggest that

$U(2n)$ breaks only for $n < n_{\text{crit}}$, where $n_{\text{crit}} \approx 3.28$. A similar value for n_{crit} is reported in a recent numerical simulation of noncompact QED.¹⁹ Since perturbative expansions of compact and noncompact QED are identical up to irrelevant terms that do not alter the low-energy behavior, the Schwinger-Dyson calculation also applies to the compact theory. However, nonperturbative effects due to the instanton gas may be important. Furthermore, the conclusion that $n_{\text{crit}} < \infty$ for noncompact QED remains controversial.

$SU(n)$ antiferromagnets can be described by compact $U(1)$ gauge theories on a spatial lattice. In particular, the flux phase of one particular two-dimensional square-lattice nearest-neighbor $SU(n)$ antiferromagnet contains massless relativistic fermions that live in the fundamental representation of $U(2n)$.³ (The two Fermi points due to lattice doubling combine, in the continuum approximation, with the n species of fermions to produce $2n$ flavors.) Again an expansion in powers of $1/n$ (holding $\alpha \equiv ne^2$ fixed) organizes the infrared divergences. The gauge fields acquire dynamics from the fermions. In particular, the leading-order term in the one-loop effective action is $(\alpha/8) |\mathbf{p}| P_{\mu\nu} A^\mu A^\nu$, where $P_{\mu\nu} \equiv \delta_{\mu\nu} - p_\mu p_\nu / \mathbf{p}^2$ and \mathbf{p} is the three-momentum. Note that the coefficient of this term is finite. Anharmonic terms, though infrared divergent, are suppressed by powers of α/n . Higher-derivative terms also appear but do not affect the infrared critical behavior of the Schwinger-Dyson equations.¹⁸ Unlike the boson antiferromagnet of Ref. 1, instantons are not adiabatic processes in the flux phase (since the spectrum is gapless) and it is unclear whether they have a definite Berry's phase. If Berry's phase is ill-defined or zero, then instantons may not generate valence-bond order.

Indeed, valence-bond order does not arise in the physical nearest-neighbor spin- $\frac{1}{2}$ $SU(2)$ antiferromagnet; rather long-range spin order occurs.²⁰ This Néel order may correspond to the symmetry-breaking pattern $U(4) \rightarrow U(2) \otimes U(2)$. In fact, a mass term that favors up spins on one sublattice and down spins on the other realizes this pattern. In the continuum notation, this term is $m(\bar{\psi}_{1\downarrow}\psi_{1\downarrow} + \bar{\psi}_{2\downarrow}\psi_{2\downarrow}) - m(\bar{\psi}_{1\uparrow}\psi_{1\uparrow} + \bar{\psi}_{2\uparrow}\psi_{2\uparrow})$, where 1 and 2 are labels for the two Fermi points. The analysis of Ref. 16 applies to this case, and massless particle-hole bound states (mesons) should occur. These mesons are the spin waves required by Goldstone's theorem. By projecting the massive-fermion wave functions onto the physical subspace of one particle per site, the ground-state energy of the antiferromagnet can be estimated. (See Ref. 3 for an explanation of this method.) The fermion mass functions as a variational parameter and recent work²¹ finds the lowest energy to be $E \approx -0.332J$

per bond (J is the antiferromagnetic exchange energy). The optimal mass is nonzero and corresponds to a realistic sublattice magnetization of about 70% of the classical Néel value. These values are in excellent agreement with the best Monte Carlo result ($E = -0.33459J \pm 0.00005J$ and 68% sublattice magnetization) obtained on a 32×32 lattice.²⁰

Finally, assuming $n_{\text{crit}} < 4$, the ground state of the $SU(4)$ antiferromagnet with appropriate biquadratic coupling (see Ref. 3) should exhibit no long-range order. It would be interesting to test this conjecture by direct study of the spin system since it could be the first example, at finite n , of a two-dimensional gapless spin liquid, resonating-valence-bond ground state.

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