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Effective lattice models for two-dimensional quantum antiferromagnets

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We introduce a 2+1 dimensional lattice model, S_0, of N complex scalars coupled to a compact $U(1)$ gauge field as a description of quantum fluctuations in $SU(N)$ antiferromagnets. Duality maps are used to obtain a single effective action for the Néel and spin-Peierls order parameters. We examine the phases of S_0 as a function of N: the $N \to \infty$ limit can be deduced from previous work. At $N = 1$, S_0 describes monopoles and their Berry phases, spin-Peierls order, but not the Néel field: Monte-Carlo simulations show a second-order transition from a spin-Peierls phase to a Higgs phase which is the remnant of the Néel phase.

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The destruction of Néel order in $d = 2$ antiferromagnets by zero temperature quantum fluctuations is of great current interest [1]. An intriguing possibility that has emerged from large-N [2, 3] expansions of unfrustrated $SU(N)$ antiferromagnets, and from numerical [4] and series [5] work on weakly frustrated antiferromagnets, is that for certain values of the spin S (all except $S = 2, 4, 6 \ldots$ for the square lattice) the disordered phase has a broken lattice symmetry and long-range spin-Peierls order. However questions on the nature of the transition between the Néel and spin-Peierls phase and the possibility of a coexistence phase have not been settled. As a first step towards resolving these issues, we introduce here a lattice effective action S_0 which describes spin fluctuations in $d = 2$ $SU(N)$ quantum antiferromagnets in terms of N complex scalars and a compact $U(1)$ gauge field. S_0 will be shown to have the following properties: *(i)* Using duality we obtain from S_0 an action S_f expressed solely in terms of the physical Néel and spin-Peierls order parameters: S_f is the correct generalization of the popular non-linear sigma ($NL\sigma$) model [6] which focuses exclusively on the Néel order. *(ii)* In the limit $N \to \infty$, previous results [3] can be used to determine the phases of S_0; the results are summarized in Fig 1a. *(iii)* Further duality transforms are used to map S_f onto an effective action, S_d, for monopole-like instantons. *(iv)* At $N = 1$ the Néel order parameter is not present but the form of the monopole interactions, their Berry phases, and the spin-Peierls order parameter survive; this limit is therefore a tractable testing ground for studying the latter effects. Results of Monte-Carlo simulations on S_f for $N = 1$ are summarized in Fig 1b. Finally, we speculate on the implication of these results for the physically relevant case of $N = 2$.

We begin by introducing S_0 as an encapsulation of previous studies [3, 6, 7, 8] of $d = 2$ $SU(N)$ antiferromagnets: we have discretized the imaginary time (τ) direction and the fields therefore lie on the sites, links and faces of a cubic lattice. We have $S_0 = S_Z + S_A + S_B$ with

$$S_Z = -\frac{N}{2g}\sum_i Z^*_{i\alpha} e^{iA_{i\mu}} Z_{i+\hat{\mu},\alpha} + h.c.\ ;\ \ S_A = \frac{N}{2e^2}\sum_i (\epsilon_{\mu\nu\lambda}\triangle_\nu A_\lambda - 2\pi q_\mu)^2\ ;\ \ S_B = i\frac{\pi}{2}\sum_{\bar{\imath}} \zeta_{\bar{\imath}} \triangle_\mu q_{\bar{\imath}\mu} \tag{1}$$

The sums over i ($\bar{\imath}$) extend over the vertices of the direct (dual) cubic lattice with the i ($\bar{\imath}$) dependence of the fields often not explicitly displayed; μ, ν, λ extend over the directions x, y, τ and $\triangle_\mu$ is the lattice derivative. All fields on the sites or links of the direct (dual) lattice have upper (lower) case letters. S_Z is a lattice version of the CP^{N-1} action [9] with Z_α a N-component complex scalar of fixed unit length ($\sum_\alpha |Z_\alpha|^2 = 1$) and $-\pi < A_\mu < \pi$ a compact U(1) gauge field. In the continuum, the CP^{N-1} model is equivalent to a $NL\sigma$ model which has been previously used [6] as a long wavelength description of $SU(N)$ antiferromagnets. For $N = 2$, Z_α is related to the Néel order parameter $\mathbf{n}$ by $\mathbf{n} = Z^*_\alpha \vec{\sigma}_{\alpha\beta} Z_\beta$ where $\vec{\sigma}$ are the Pauli matrices. S_A is the kinetic energy of A_μ in a periodic gaussian form: q_μ is integer valued field on the links of the dual lattice. Although no such term is present in the bare CP^{N-1} model, it will always be dynamically generated *e.g.* by integrating out the Z_α bosons between momentum scales Λ and $\Lambda/2$ where $\Lambda \sim 1/a$ is the upper cutoff. S_B is the crucial Berry phase [7, 3] for antiferromagnets with spins in the fundamental representation of $SU(N)$ on one sublattice and in the conjugate representation on the other (for $N = 2$ both correspond to spin $S = 1/2$); we will consider this value of the spin exclusively. The *fixed* field $\zeta_{\bar{\imath}}$ is τ independent and has the values $0, 1, 2, 3$ on dual lattice sites with even-even, even-odd, odd-odd, and odd-even spatial co-ordinates (Fig 2). The quantity $\triangle_\mu q_\mu$ is the divergence of the $U(1)$ flux and equals the number of Dirac monopoles. For *small* e^2 and $A_\mu = A^D_\mu$, the vector potential of a Dirac monopole with total flux 2π, the action will be minimized with $q_\mu = 1$ along the Dirac string; $\triangle_\mu q_\mu$ is thus the number operator for the monopoles. The monopoles are closely tied to the 'hedgehogs' in the Néel field (see Ref [3] and below) which were first shown by Haldane [7] to carry Berry phases. For $e^2 \to \infty$ the fluctuations of q_μ and A_μ are less strongly coupled; in fact at $e^2 = \infty$ the sum over q_μ is trivial and we obtain $\mathrm{Tr} e^{-S_0} = 0$! The large e^2 limit must therefore be taken with some care and we shall show below that the proper Berry phase continues to be associated with each monopole. We will consider properties of S_0 as a function of e^2 and g for all $N \geq 1$; for $N = 1$ S_0 describes a Higgs scalar coupled to a compact $U(1)$ gauge field whose monopoles carry Berry phases. The analyses for all $N \geq 2$ are very similar; we will therefore often present explicit results only for $N = 1, 2$.

Standard duality methods [10] can be used to exchange the summation over q_μ for summation over an integer valued field a_μ lying on the links of the dual lattice. This transforms S_0 into

$$S_1 = \frac{e^2}{2N} \sum_{\bar{\imath}} \left(a_\mu - \frac{1}{4} \triangle_\mu \zeta \right)^2 + i \sum_i A_\mu \epsilon_{\mu\nu\lambda} \triangle_\nu a_\lambda - \frac{N}{2g} \sum_i Z^*_{i\alpha} e^{iA_{i\mu}} Z_{i+\hat{\mu},\alpha} + h.c. \qquad (2)$$

Correlations of the integer-valued dual 'flux' [11] $\epsilon_{\mu\nu\lambda} \triangle_\nu a_\lambda$ under S_1 are identical to those of the Z_α boson current under S_0. Conversely, the $U(1)$ fluxes $(\epsilon_{\mu\nu\lambda} \triangle_\nu A_\lambda - 2\pi q_\mu)$ are dual to $e^2 (a_\mu - \triangle_\mu \zeta / 4)$; in particular, the spin-Peierls order parameters, Ψ_x, Ψ_y, were shown in Ref. [3] to be proportional to the electric field. We therefore identify [12]

$$\Psi_p = \frac{e^2}{N_s} \epsilon_{pq} \sum_{\bar{\imath}} (-1)^{\bar{\imath}_x + \bar{\imath}_y} \left(a_{\bar{\imath}q} - \frac{1}{4} \triangle_q \zeta_{\bar{\imath}} \right) \qquad (3)$$

where N_s is the number of sites, $p, q = x, y$, and the four possible signs of the pair Ψ_x, Ψ_y identify the four spin-Peierls states (Fig 2).

The large e^2 limit is straightforward with S_1. The a_μ fields are frozen at $a^0_\mu = \aleph(\triangle_\mu \zeta / 4)$ where $n = \aleph(x)$ is the integer nearest to x (because $a^0_\mu \neq \triangle_\mu \zeta / 4$, $\mathrm{Tr} e^{-S_1} \propto \exp(-c e^2) \to 0$ as $e^2 \to \infty$; this prefactor will however cancel out of all correlation functions). Using the result $\epsilon_{\mu\nu\lambda} \triangle_\nu a^0_\lambda = \delta_{\mu\tau} (-1)^{i_x + i_y}$ the imaginary term in S_1 becomes $i \sum_i (-1)^{i_x + i_y} A_\tau$. For $A_\mu = A^D_\mu$

the summation over i is exactly that evaluated by Haldane [7] and thus yields the same monopole Berry phase.

It is now useful to introduce the parametrization $\sum_\alpha Z^*_{i\alpha} Z_{i+\hat{\mu},\alpha} \equiv Q_{i\mu}\exp(i\mathcal{A}_{i\mu})$ with $Q_{i\mu}$ real, positive and $-\pi < \mathcal{A} < \pi$, We note that for $N=1$, $Q_{i\mu}=1$ while for $N=2$, $Q_{i\mu} = ((1+\mathbf{n}_i\cdot\mathbf{n}_{i+\hat{\mu}})/2)^{1/2} \approx 1 - a^2(\partial_\mu \mathbf{n}_i)^2/8$ where a is the lattice spacing. The functional integral over A_μ in S_1 can be performed and yields a product of modified Bessel functions of $Q_{i\mu}/g$. As is conventional [10] the Bessel functions are replaced by their large argument expansion yielding finally (for $N=2$) the partition function $Z = \int \mathcal{D}\mathbf{n} \sum_{a_\mu} e^{-S_f}$ with $S_f = S_a + S_\mathbf{n} + S_c$ and

$$\begin{aligned} S_a &= \frac{e^2}{2N}\sum_{\bar{\imath}}\left(a_\mu - \frac{1}{4}\triangle_\mu \zeta\right)^2 + \frac{g}{2N}\sum_{\bar{\imath}}(\epsilon_{\mu\nu\lambda}\triangle_\nu a_\lambda)^2 \\ S_\mathbf{n} &= \frac{1}{4ga}\int d^3r(\partial_\mu \mathbf{n})^2 + \ldots \quad ; \quad S_c = -2\pi i \sum_{\bar{\imath}} a_\mu k_\mu(\mathbf{n}) \end{aligned} \tag{4}$$

where the ellipses denote *real* higher-order terms that are generated by the expansion of the Bessel function. The variable $k_\mu(\mathbf{n})$ is the topological current of $\mathbf{n}$ [9]

$$k_\mu(\mathbf{n}) \equiv \frac{1}{2\pi}\epsilon_{\mu\nu\lambda}\triangle_\nu \mathcal{A}_\lambda = \frac{1}{4\pi}\Omega(\mathbf{n}_i, \mathbf{n}_{i+\hat{\mu}}, \mathbf{n}_{i+\hat{\mu}+\hat{\nu}}, \mathbf{n}_{i+\hat{\nu}}) \approx \frac{a^2}{4\pi}\epsilon_{\mu\nu\lambda}\mathbf{n}\cdot(\partial_\nu \mathbf{n} \times \partial_\lambda \mathbf{n}) \tag{5}$$

where $\Omega(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3, \mathbf{n}_4)$ is the area of the spherical cap spanned by $\mathbf{n}_1 \ldots \mathbf{n}_4$; the second equality is only true upto an integer which leaves Z unchanged. S_f is the advertised action controlling the fluctuations of the spin-Peierls and Néel order. For $N=2$ the mapping between S_0 and S_f is similar in spirit to analyses in Ref [13] for the quantum Hall effect. For $N=1$, there is no Néel order parameter; thus $S_c = S_\mathbf{n} = 0$ and $S_f = S_a$.

We now examine the properties of S_0 and S_f in different parameter regimes:

1. $\mathbf{e^2} \to \infty$: The a_μ fields are frozen at $a^0_\mu = \aleph(\triangle_\mu \zeta/4)$; S_c can then be shown to equal $i\sum_i (-1)^{i_x+i_y}\mathcal{A}_\tau$. This is identical to the individual spin Berry phase found in Ref [7] as, in an appropriate gauge, $\mathcal{A}_\tau(i)$ is half the solid angle between $\mathbf{n}(i)$, $\mathbf{n}(i+\hat{\tau})$ and $\hat{\mathbf{z}}$. *Remarkably,* *the monopole Berry phase has uniquely fixed the individual spin Berry phases;* the resulting action for $\mathbf{n}$ is thus identical to that of Ref [7]. For $N = 1$, the quenching of a_μ rules out the possibility of a phase transition at $e^2 = \infty$.

2. $\mathbf{e^2 = 0}$: The A_μ field is pure gauge and we choose $A_\mu = q_\mu = 0$. The action S_0 is simply that of a *classical* three dimensional $U(N)$ spin model which has a second-order phase transition $g = g_c$ with exponent [14] $\nu = 1/2 + \epsilon(N+1)/(4(N+4)) + \ldots$ where $\epsilon = 4 - D = 1$. The action $S_f(e^2 = 0)$ is an unconventional representation of this well-known model. Following Peskin [15], it can be shown that [16] the two phases of the $U(N)$ model can be characterized by different asymptotic limits of correlation functions of a_μ alone: the small g phase has a proliferation of macroscopic loops of the Z_α boson current $\epsilon_{\mu\nu\lambda}\triangle_\nu a_\lambda$, which are absent in the large g phase.

3. Small $\mathbf{e^2}$: The concentration of monopoles is exponentially small ($\sim \exp(-cN/e^2)$); we now show that for *all* values of N oppositely charged monopoles have a bare linear attraction $\sim NR/g$ for small g and a Coulombic $N/(e^2R)$ attraction at large g. The monopole effective interaction is obtained by promoting the sum over a_μ into an integral by the Poisson method; this produces an integer-valued field $v_{\bar{\imath}\mu}$ residing on the links of the dual lattice which is the vorticity in the Z_α boson current. Integrating over a_μ we get $Z = \int \mathcal{D}\mathbf{n} \sum_{v_\mu} \exp(-S_d)$ with

$$S_d = 2\pi^2 \sum_{\bar{\imath},\bar{\jmath}} \left((v_{\bar{\imath}\mu} + k_{\bar{\imath}\mu}) G(\bar{\imath} - \bar{\jmath}) (v_{\bar{\jmath}\mu} + k_{\bar{\jmath}\mu}) + \frac{g}{e^2} m_{\bar{\imath}} G(\bar{\imath} - \bar{\jmath}) m_{\bar{\jmath}} \right) + i\frac{\pi}{2} \sum_{\bar{\imath}} m_{\bar{\imath}} \zeta_{\bar{\imath}} + S_{\mathbf{n}} \qquad (6)$$

where $G(r)$ is the Green's function of the lattice Helmholtz equation $(-g\triangle^2 + e^2)G(r) = N\delta(r)$. We have used $\triangle_\mu k_\mu = 0$ and introduced the monopole density $m = \triangle_\mu v_\mu$: the monopoles thus terminate lines of vorticity and carry the Berry phase $\pi\zeta/2$. We now examine the v_μ, k_μ fluctuations for a fixed monopole density for large and small g *(i) Small* g: Now $G(0) \sim N/g$ is large and for $N = 2$, S_d forces the minimization of $v_\mu + k_\mu$ as in Fig 3; each monopole is thus bound a hedgehog in the $\mathbf{n}$ field. The action for Fig 3 arises predominantly from $S_{\mathbf{n}}$ and yields [17] to yield a attractive potential $\sim NR/g$ where R is the separation of the monopoles. For $N = 1$, $k_\mu = 0$; the action for each monopole-anti-monopole pair is given by that of the v_μ string connecting them $\sim G(0)R \sim R/g$. *(ii) Large g* The v_μ and k_μ fluctuations are less strongly coupled. We integrate out the $\mathbf{n}$ fluctuations in S_f (Eqn 4) by a 'high-temperature' expansion and sum over v_μ (subject to the constraint $\triangle_\mu v_\mu = m$) in a Debye-Huckel approximation [18]. This can be shown to yield [16] an effective Coulombic interaction $\sim N m_{\bar{\imath}} m_{\bar{\jmath}}/(e^2|r_{\bar{\imath}} - r_{\bar{\jmath}}|)$ between monopole charges [3] for all N.

4. Large g: The $\mathbf{n}$ fluctuations can be integrated out in a 'high temperature' expansion and, apart from an innocuous renormalization of parameters, the physics is independent of N. The results can therefore be deduced from the $N = 1$ case.

We now turn to a detailed study of $N = 1$ for which $S_f = S_a$. For $g = \infty$, a_μ is restricted to $a_\mu = \triangle_\mu \chi$ where χ is an integer-valued scalar field; S_a is now equivalent [3] to the discrete Gaussian model of Ref. [19] obtained via a duality transform on a quantum-dimer representation of the disordered phase of quantum antiferromagnets. Numerical simulations on this model have been carried out [20] and are consistent with our results below. For $g \neq \infty$ it is useful to examine the global minima of S_a. We find two regimes: *(i)* $g < e^2/4$: The lowest action states have $a^0_\mu = \aleph(\triangle_\mu \zeta/4)$ which implies $\Psi^0_p = 0$. *(ii)* $g > e^2/4$: Now $a^0_\mu = \triangle_\mu \chi^0$. There is however a large degeneracy in the choice of χ^0 with one state being associated with every dimer close-packing of the square lattice.

We have performed Monte-Carlo simulations on S_a to study the effects of fluctuations. The standard Metropolis algorithm was used with 3×10^5 time steps per site. Long equilibration times restricted us to $e^2 \leq 6$. The results are summarized in Fig 1b. We find two phases: *(i)* a large g spin-Peierls phase where fluctuation effects lead to crystallization of the dimers in columns (Fig 2); at $g = \infty$ spin-Peierls order is expected to exist for all finite

e^2 [3] *(ii)* a small g Higgs phase in the $U(1)$ scalar Z_α. A scaling plot of the invariant ratio $r = \langle(\Psi_x^2 + \Psi_y^2)^2\rangle / \langle(\Psi_x^2 + \Psi_y^2)\rangle^2$ (Fig 4) shows clearly that the phase transition at $e^2 = 2.0$ is continuous; we find the exponents $\nu = 0.64 \pm 0.05$ and the specific heat peak [16] is consistent with $\alpha \approx 0$. The Z_4 lattice symmetry breaking pattern of the spin-Peierls states suggests that the phase transition is in the universality class of the $D = 3$, Z_4 clock model, or equivalently, the two-color Ashkin Teller model. The second-order transition in the latter model is XY-like [21] and the exponents $\nu_{XY} \approx 2/3$ and $\alpha_{XY} \approx 0$ are consistent with our results. We recall that the phase transition at $e^2 = 0$ is also XY-like but with the small g phase being the ordered one.

The analysis of S_0 and S_f for the important $N = 2$ case is complicated by the imaginary term whose form suggests a 'dual' relationship between the Néel and spin-Peierls ordering. We have just argued that for large g, spin-Peierls order will be present. At small g the $\mathbf{n}$ field will order; a spin-wave analysis of S_c shows that $\mathbf{n}$ fluctuations induce a power-law coupling in the a_μ field: $\sim g^2(\vec{\triangle} \times \vec{a})_{i\mu}(1/r^4)(\delta_{\mu\nu} - 3r_\mu r_\nu/r^2)(\vec{\triangle} \times \vec{a})_{j\mu}$ where $r = r_i - r_j$. This coupling will favor fluctuations in the local value of $\vec{\triangle} \times \vec{a}$; the spin-Peierls states have $\vec{\triangle} \times \vec{a} = 0$ and will therefore be suppressed although we cannot rule out coexistence between the Néel and spin-Peierls phases. Conversely, the existence of an intermediate phase with neither Néel or spin-Peierls ordering is not possible at $e^2 = 0$, and has been argued [3] to be unlikely when the monopole concentration ($\sim \exp(-cN/e^2)$ for S_0) is small. A possible scenario is therefore a single phase boundary coming in at a finite value of g as $e^2 \to \infty$; unlike $N \to \infty$ (Fig 1a) however, the phase boundary will not be vertical. Monte-Carlo or other analyses of the actions S_0 or S_f for $N = 2$ to resolve these questions is clearly an important subject for future research.

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the co-efficient of e^2 to $(a_\mu - \triangle_\mu \phi - \triangle_\mu \zeta/4)^2$. The expression (2) for S_1 corresponds to the gauge choice $\phi = 0$ which has been implicitly made in this paper.

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Figure Captions

1. Phase diagrams of the effective action S_0, and its dual S_f. The $N \to \infty$ result was deduced from Ref [3], the $N = 1$ result from our Monte-Carlo simulations. The phase transition at $e^2 = 0$ is that of a classical three-dimensional $U(N)$ spin model and is thus second-order. For finite e^2, the transition is second-order *at* $N = \infty$; its behavior for finite but large N is unknown. For $N = 1$ we observed a transition at the points shown (the line is a guide to the eye and is theoretically expected to go into the point $(e^2 = \infty, g = \infty)$); the scaling analysis in Fig 4 for $e^2 = 2.0$ shows that the transition is second-order. In the limit $g \to \infty$ the model is insensitive to N and is equivalent to the discrete Gaussian model of Fradkin and Kivelson [19] obtained via a duality transform on the quantum dimer model.

2. Fully ordered spin-Peierls state. The numbers denote values of the *fixed* field ζ and the fluctuating field a_μ lies on the arrows. Each dimer covering corresponds to a value of $a_\mu - (\triangle_\mu \zeta)/4$ of $-3/4$ across dimerized links and of $1/4$ across all other links. The particular dimerization shown therefore has $a_\mu = 0$.

3. A pair of point defects at small g showing the binding between monopoles and hedgehogs.

4. Scaling plot of the invariant ratio $r = \langle(\Psi_x^2 + \Psi_y^2)^2\rangle / \langle(\Psi_x^2 + \Psi_y^2)\rangle^2$ at $N = 1$ and $e^2 = 2.0$ for lattices with L^3 sites. As $g \to \infty$ (the spin-Peierls phase), $r \to 1$ while as $g \to 0$, $r \to 2$ which corresponds to gaussian fluctuations about $\Psi_p = 0$. The fitting parameters are $\nu = 0.64 \pm 0.05$ and $g_c = 2.39$.

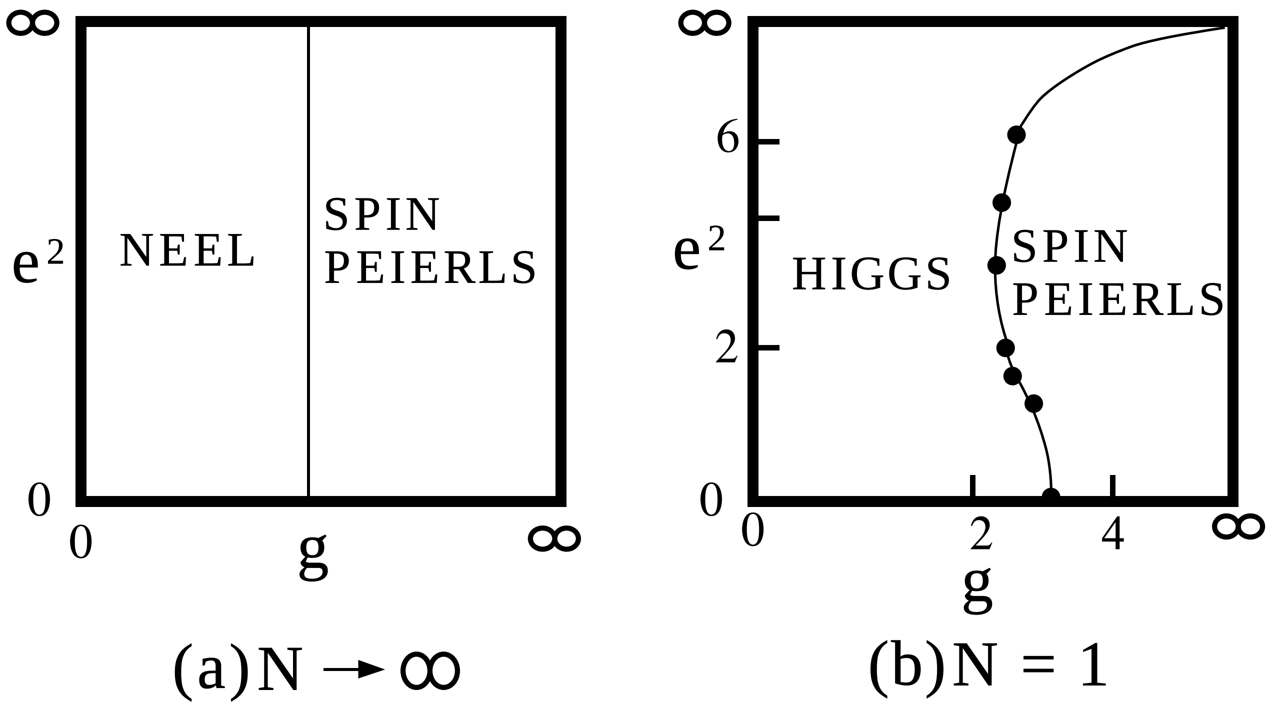
∞
e²
0
0
g
∞
NEEL
SPIN
PEIERLS
(a) N → ∞
∞
6
e²
2
0
0
2
4
∞
g
HIGGS
SPIN
PEIERLS
(b) N = 1

Figure 1

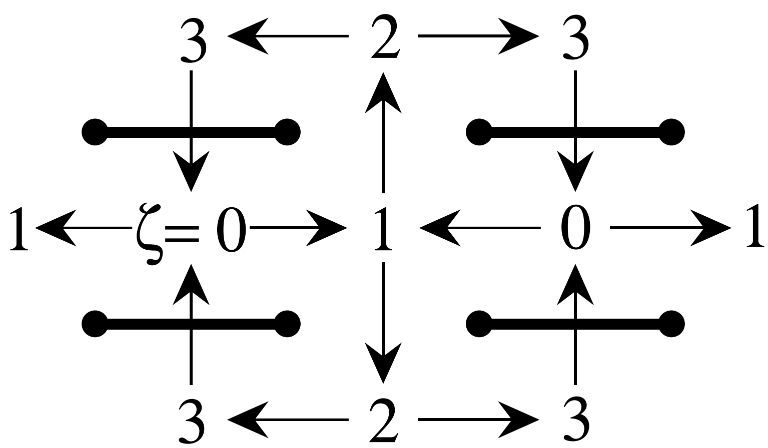

Figure 2

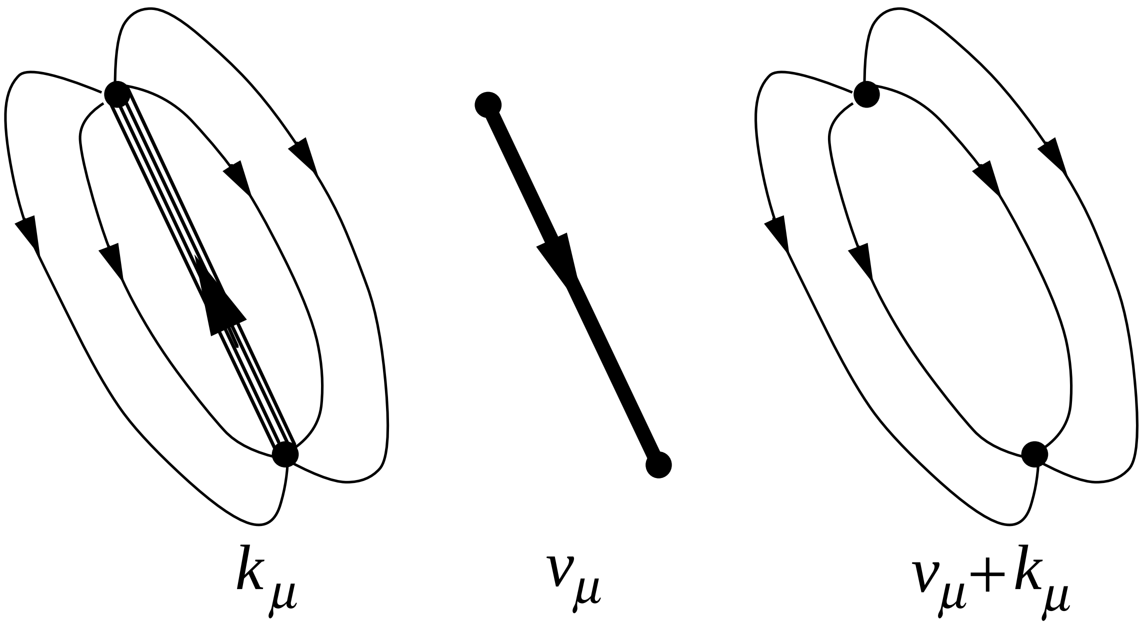

Figure 3

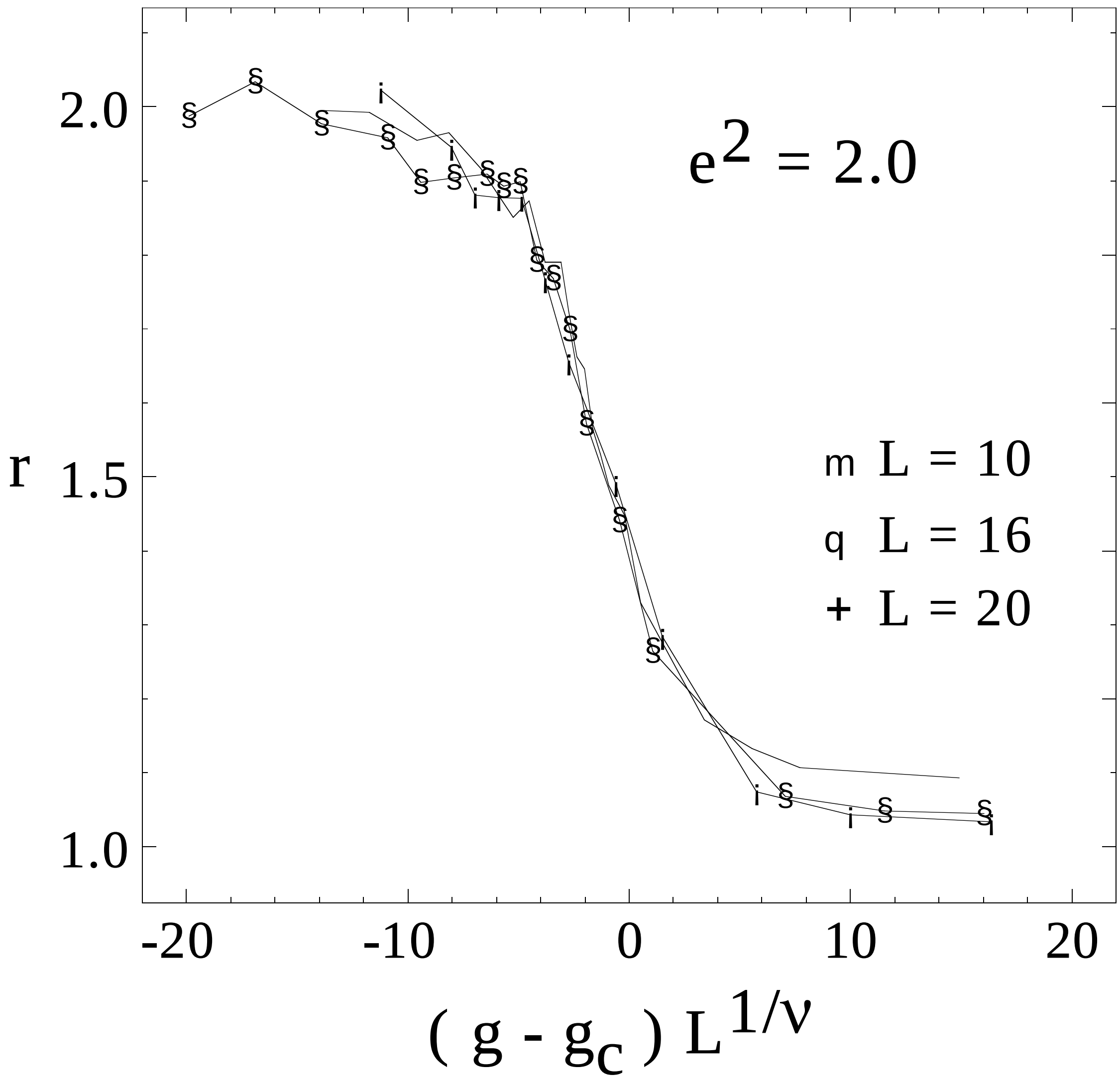

Figure 4