

Quantum Nonlinear σ Model for Arbitrary Spin Heisenberg Antiferromagnets

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We derive a quantum nonlinear sigma model (QNLSM) for quantum Heisenberg antiferromagnets (QHA) with arbitrary S (spin) values. An upper limit of the low temperature is naturally carried out for the reliability of the QNLSM. The S dependence of the effective coupling constant and the spin-wave velocity in the QNLSM are also obtained explicitly. The resulting spin-wave velocity for 2D spin-1/2 QHA highly concurs with the experimental data of high T_c compound La_2CuO_4 . The predicted correlation lengths for 2D QHA and spin-gap magnitudes for 1D QHA also agree with the accurate numerical results.

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Quantum magnetism in low-dimensional strongly correlated systems is a central issue in modern condensed matter physics. For example, the parent compounds of the cuprate high T_c superconductors are essentially antiferromagnetic Mott insulators described by a two-dimensional spin- $\frac{1}{2}$ quantum Heisenberg antiferromagnets (QHA) [1]. Such a low-dimensional QHA system has not been fully solved quantum mechanically. Only in the *large S limit* has Haldane shown that the lattice QHA can be described by the quantum nonlinear sigma model (QNLSM) [2]. Since then, the QNLSM has become a good candidate for the *phenomenological* description of the low-dimensional QHA at low temperatures for various S values [3–5].

However, two crucial questions remain for the QNLSM approach: (1) Why are the predictions of QNLSM obtained in the large- S limit coincidentally consistent with experimental data of the low energy QHA with small S values? and (2) What is the upper limit of the low temperature for the reliability of QNLSM? These two questions, along with other difficulties for the QNLSM, have been addressed in some recent literatures [6]. But they have not yet been satisfactorily solved in a simple, consistent approach. In this Letter, with the topologically invariant spin variable path integral approach, we resolve these problems by deriving a QNLSM from the lattice QHA for arbitrary S values.

Let us first briefly recall the large- S approach of the QNLSM. The partition function of a spin system is usually expressed in terms of the spin variable path integral as follows (in the unit $\hbar = k_B = 1$):

$$Z = \text{Tr} e^{-\beta H} = \int \mathcal{D}[\mathbf{\Omega}] e^{\int_0^\beta d\tau \{iS \mathbf{A} \cdot \dot{\mathbf{\Omega}} - \langle \mathbf{\Omega} | H | \mathbf{\Omega} \rangle\}}, \quad (1)$$

where the first term in the exponent $iS \int_0^\beta d\tau \mathbf{A} \cdot \dot{\mathbf{\Omega}} = \int_0^\beta d\tau \langle \mathbf{\Omega} | \frac{d}{d\tau} | \mathbf{\Omega} \rangle \equiv iS \omega(\mathbf{\Omega})$ is a topological Berry phase [7], and \mathbf{A} is a U(1) monopole potential; $|\mathbf{\Omega}\rangle$ is a spin coherent state while $\mathbf{\Omega}$ is a unit vector along which the spin operator with spin quantum number S is maximally aligned in $|\mathbf{\Omega}\rangle$. For the lattice Heisenberg model (HM), $H =$

$J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$ ($J > 0$), Eq. (1) becomes

$$Z_H = \int \mathcal{D}[\mathbf{\Omega}_i] e^{\int_0^\beta d\tau \{iS \sum_i \mathbf{A}_i \cdot \dot{\mathbf{\Omega}}_i - JS^2 \sum_{\langle ij \rangle} \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j\}}. \quad (2)$$

By minimizing $H(\mathbf{\Omega}) = JS^2 \sum_{\langle ij \rangle} \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j$, one can find the classical ground state (Néel state) which spontaneously breaks the SO(3) symmetry. Then by expanding the action around the ground state, the spin-wave theory of HM, which describes the long wavelength spin modes [8], can be easily derived.

But, according to the Mermin-Wagner's theorem [9], no symmetry can be spontaneously broken in one- or two-dimensional HM for a finite T (> 0). To derive an effective long wavelength action that retains the full spin rotational symmetry, Haldane considered the large- S limit. In the large- S limit, the path integrals of Eq. (2) are dominated by the semiclassical equation: $iS \mathbf{\Omega} \times \dot{\mathbf{\Omega}} = \frac{\partial H[\mathbf{\Omega}]}{\partial \mathbf{\Omega}}$. By separating the semiclassical solution $\mathbf{\Omega}_i$ into a slowly varying Néel order unit vector $(-1)^i \mathbf{n}(x_i)$ plus a slowly varying magnetization density field perpendicular to $\mathbf{n}(x_i)$ (Haldane's mapping), and then taking the continuous limit and integrating out the magnetic density field, Haldane shows that Eq. (2) is reduced to a QNLSM,

$$Z_H = \int \mathcal{D}[\mathbf{n}] e^{i2\pi S \Theta[\mathbf{n}]} e^{-(\Lambda^{d-1}/2g_o) \int d^{d+1}x \partial_\mu \mathbf{n} \partial^\mu \mathbf{n}}, \quad (3)$$

defined in the $(d+1)$ -dimensional space $(x^1, \dots, x^{d+1}) = (x^1, \dots, x^d, c_o \tau)$ where $g_o = 2\sqrt{d}/S$ is a dimensionless coupling constant, $c_o = 2\sqrt{d}JSa$ the spin-wave velocity and $\Lambda = a^{-1}$ the inverse of the lattice spacing. The imaginary time (temperature) variable τ ranges from 0 to $\beta = 1/T$. The exponent $\Theta[\mathbf{n}]$ in Eq. (3) is a topological factor associated with the Berry phase.

However, as we will elaborate, the derivation of the QNLSM based on the large- S expansion should be improved from the very beginning. As a long-standing problem in the construction of generalized phase space path integrals [10], the Eq. (1) is not well defined. The main problem arises from the assumption, used in deriving

Eq. (1), that $|\mathbf{\Omega}(\tau + \delta\tau)\rangle - |\mathbf{\Omega}(\tau)\rangle$ is of order $O(\delta\tau)$. Although this assumption has been widely used in the application of generalized phase space path integrals, it has never been justified [10]. In fact, in effective field theories, there always exist simultaneous rapidly and slowly varying paths in the path integral formalism that are associated with short and long range quantum fluctuations, respectively. The effective action for slowly varying motions can be properly obtained by integrating over short range quantum fluctuations [11]. However, in Eq. (1), only slowly varying motions are retained; the short range quantum fluctuations have simply been ignored.

To overcome the shortcomings involved in the derivation of Eq. (1), we begin with the discrete form of the partition function obtained exactly from the coherent state representation [12]:

$$Z = \lim_{N \rightarrow \infty} \prod_{k=1}^N d\mu(\mathbf{\Omega}^k) \exp \left\{ \sum_{k=1}^N \ln \langle \mathbf{\Omega}^k | \mathbf{\Omega}^{k-1} \rangle - \epsilon \frac{\langle \mathbf{\Omega}^k | H | \mathbf{\Omega}^{k-1} \rangle}{\langle \mathbf{\Omega}^k | \mathbf{\Omega}^{k-1} \rangle} \right\} \quad (4)$$

(where $|\mathbf{\Omega}^N\rangle = |\mathbf{\Omega}^0\rangle$ because of the periodicity of the trace), $\epsilon = \beta/N$ is infinitesimal as $N \rightarrow \infty$. The slowly varying motion means that $|\mathbf{\Omega}_i\rangle - |\mathbf{\Omega}_{i-1}\rangle$ varies smoothly in the interval ϵ such that it can be written as a time derivative $\epsilon|\dot{\mathbf{\Omega}}\rangle$. The rapidly varying motion of $|\mathbf{\Omega}_i\rangle - |\mathbf{\Omega}_{i-1}\rangle$ in the interval ϵ is related to the short range quantum fluctuations; we label it as $\delta\mathbf{\Omega}$. The assumption of $|\mathbf{\Omega}^k\rangle - |\mathbf{\Omega}^{k-1}\rangle$ being of order $O(\epsilon)$ only keeps the slowly varying motions $\dot{\mathbf{\Omega}}$, while the short range fluctuations $\delta\mathbf{\Omega}$ is ignored. Thus, the continuous-time limit of (4) results in the conventional spin variable path integral of Eq. (1).

To include the contribution of the short range fluctuations, one should expand the nearby coherent state overlap to the second order terms that either are exclusively slowly varying motions or include at least one rapidly varying motion. The topologically invariant terms $\lim_{N \rightarrow \infty} \sum_{k=1}^N \ln \langle \mathbf{\Omega}^k | \mathbf{\Omega}^{k-1} \rangle$ can then be uniquely expressed by

$$S \int_0^\beta d\tau \left\{ i\mathbf{A} \cdot \dot{\mathbf{\Omega}} + i\mathbf{\Omega} \cdot (\dot{\mathbf{\Omega}} \times \delta\mathbf{\Omega}) - \frac{1}{\tau_\Lambda} \delta\mathbf{\Omega} \cdot \delta\mathbf{\Omega} \right\}, \quad (5)$$

where the parameter $\tau_\Lambda \equiv 1/T_\Lambda$ is an intrinsic shortest time scale (an upper limit of low temperature) for distinguishing the slowly varying and rapidly varying motions. We will later discuss this time scale in detail. The second and third terms in Eq. (5) are usually ignored in the conventional derivation of phase space path integrals. For the Hamiltonian term in Eq. (4), $\lim_{N \rightarrow \infty} \sum_{k=1}^N \epsilon \frac{\langle \mathbf{\Omega}^k | H | \mathbf{\Omega}^{k-1} \rangle}{\langle \mathbf{\Omega}^k | \mathbf{\Omega}^{k-1} \rangle}$, since it is already proportional to ϵ we only keep the off-diagonal expansion up to the quadratic order of $\delta\mathbf{\Omega}$:

$$\int d\tau \left\{ H[\mathbf{\Omega}] + \frac{\partial H[\mathbf{\Omega}]}{\partial \mathbf{\Omega}} \cdot \delta\mathbf{\Omega} + \frac{\partial^2 H[\mathbf{\Omega}]}{\partial \mathbf{\Omega}_\alpha \partial \mathbf{\Omega}_{\alpha'}} \delta\mathbf{\Omega}_\alpha \delta\mathbf{\Omega}_{\alpha'} \right\}, \quad (6)$$

where α, α' are indices of spin components. Substituting Eqs. (5) and (6) into Eq. (4), one gets

$$Z = \int \mathcal{D}[\mathbf{\Omega}] \mathcal{D}[\delta\mathbf{\Omega}] \exp \int_0^\beta d\tau \left\{ iS\mathbf{A} \cdot \dot{\mathbf{\Omega}} - H[\mathbf{\Omega}] + \left[iS\mathbf{\Omega} \times \dot{\mathbf{\Omega}} - \frac{\partial H[\mathbf{\Omega}]}{\partial \mathbf{\Omega}} \right] \cdot \delta\mathbf{\Omega} - \left[\frac{S}{\tau_\Lambda} \delta_{\alpha\alpha'} + \frac{\partial^2 H[\mathbf{\Omega}]}{\partial \mathbf{\Omega}_\alpha \partial \mathbf{\Omega}_{\alpha'}} \right] \delta\mathbf{\Omega}_\alpha \delta\mathbf{\Omega}_{\alpha'} \right\}, \quad (7)$$

which describes both the slowly varying motion $\dot{\mathbf{\Omega}}$ and the short range fluctuations $\delta\mathbf{\Omega}$.

If one takes the semiclassical limit, $iS\mathbf{\Omega} \times \dot{\mathbf{\Omega}} - \frac{\partial H[\mathbf{\Omega}]}{\partial \mathbf{\Omega}} = 0$, Eq. (7) is simply a variation expansion of the path integral (1) with respect to the semiclassical dynamics Haldane used [2], except for the geometrical term $\frac{S}{\tau_\Lambda}$ which cannot appear in Haldane's mapping. However, we must emphasize that Eq. (7) is derived by carefully treating the off-diagonal elements of nearby coherent states in Eq. (4) in terms of the short range fluctuation $\delta\mathbf{\Omega}$ and the slowly varying motions $\dot{\mathbf{\Omega}}$. Since there is no semiclassical expansion to begin with, it is not necessary to take the semiclassical limit by letting the second term vanish. Instead, one can integrate out the short range fluctuations $\delta\mathbf{\Omega}$ and obtain a low energy effective action for the long wavelength spin modes. Since no semiclassical approximation is made in this procedure, the resulting long wavelength effective action should be valid for arbitrary S values.

Next, we apply Eq. (7) to the HM. To specify the antiferromagnetic ordering, let the slowly varying $\mathbf{\Omega}_i = (-1)^i \mathbf{n}(x_i)$; here the Néel order $\mathbf{n}(x_i)$ is a unit vector $|\mathbf{n}(x_i)| = 1$. Then, by taking the space continuous limit $\sum_i \rightarrow \frac{1}{a^d} \int d^d x$ where a is the lattice spacing:

$$H[\mathbf{\Omega}] = JS^2 \sum_{\langle ij \rangle} \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j \rightarrow -dJS^2 N + \frac{JS^2}{2a^{d-2}} \int d^d x \sum_{k=1}^d [\partial_k \mathbf{n}(x) \cdot \partial_k \mathbf{n}(x)], \quad (8)$$

$$\frac{\partial H[\mathbf{\Omega}]}{\partial \mathbf{\Omega}} \cdot \delta\mathbf{\Omega} \rightarrow 0, \quad (9)$$

$$\frac{\partial^2 H[\mathbf{\Omega}]}{\partial \mathbf{\Omega}_\alpha \partial \mathbf{\Omega}_\beta} \delta\mathbf{\Omega}_\alpha \delta\mathbf{\Omega}_\beta \rightarrow \frac{2dJS^2}{a^d} \int d^d x \delta\mathbf{\Omega}(x) \cdot \delta\mathbf{\Omega}(x). \quad (10)$$

substituting (8)–(10) into (7), and integrating out the short range fluctuation $\delta\mathbf{\Omega}$, we obtain,

$$Z_H = \int \mathcal{D}[\mathbf{n}] e^{i2\pi S \Theta[\mathbf{n}]} \exp\left\{-\frac{a^{1-d}}{2g_s} \int_{c_s/T_\Lambda}^{c_s/T} d(c_s\tau) \times \int d^d x \left[\frac{1}{c_s^2} \left| \frac{\partial \mathbf{n}}{\partial \tau} \right|^2 + |\nabla_x \mathbf{n}|^2 \right]\right\}. \quad (11)$$

This is a QNLMS of the low energy QHA for arbitrary S values, where the coupling constant and spin-wave velocity are given by

$$g_s = \frac{2}{S} \sqrt{d + \frac{T_\Lambda}{2SJ}}, \quad c_s = 2JSa \sqrt{d + \frac{T_\Lambda}{2SJ}}. \quad (12)$$

The topological phase factor $2\pi S \Theta[\mathbf{n}] = 2\pi S \sum_i (-1)^i \mathbf{A}(x_i) \cdot \dot{\mathbf{n}}(x_i)$ remains the same as in Haldane's derivation.

In the large- S limit for fixed T_Λ , $g_s \rightarrow 2\sqrt{d}/S$, and $c_s \rightarrow 2\sqrt{d}JSa$. This reproduces the large- S QNLMS. The difference between (3) and (11) primarily comes from the contribution of the short range fluctuations, the $1/\tau_\Lambda = T_\Lambda$ term in (7) which cannot be included in Haldane's mapping [2]. However, this term plays an important role in the derivation of a consistent semiclassical dynamics [13]. Indeed, T_Λ is an upper limit of the low temperature scale for the reliability of the QNLMS. Usually one assumes that there should be no intrinsic cutoff for the imaginary time variable τ because quantum fluctuations exist on all time scales in path integrals [3]. But a low energy effective theory constructed from the path integral is defined by integrating over high energy quantum fluctuations above certain energy scale [11]. Without such an intrinsic cutoff, namely, letting $\tau_\Lambda \rightarrow 0$ ($T_\Lambda \rightarrow \infty$), Eq. (11) reduces to

$$Z_H \propto \int \mathcal{D}[\mathbf{n}] e^{i2\pi S \Theta[\mathbf{n}]} \exp\left\{-\frac{\rho_s}{2T} \int [d^d x |\nabla_x \mathbf{n}|^2]\right\}, \quad (13)$$

where $\rho_s = JS^2 a^{2-d}$ is the spin stiffness. Except for the topological phase, this is the classical d -dimensional NLSM rather than a quantum $(d+1)$ -dimensional NLSM that Haldane obtained [2]. This is because in the limit $\tau_\Lambda \rightarrow 0$, the strong canonical fluctuation in Eq. (5) smears the dynamical fluctuation of Eq. (10) so that only the classical Hamiltonian Eq. (8) remains.

Now, let us discuss how to consistently determine this time scale. The lattice spacing a indicates the existence of an intrinsic momentum cutoff Λ in the d -dimensional momentum space: $\Lambda = 2\sqrt{\pi}[\Gamma(d/2 + 1)]^{1/d}/a \equiv L/a$. Using the energy-momentum relation of the spin wave, $E = c_s k$, one can find the intrinsic energy cutoff (the inverse of the shortest time scale τ_Λ) $T_\Lambda = c_s \Lambda / 2\pi$ [8]. Combined with (12), we get

$$\frac{T_\Lambda}{J} = \frac{SL^2}{4\pi^2} \left(1 + \sqrt{1 + \frac{16\pi^2 d}{L^2}} \right). \quad (14)$$

For $d = 2$ and $S = 1/2$, we have $L = 2\sqrt{\pi}$ and thus $T_\Lambda/J \approx 0.97$. This determines quantitatively a low tem-

perature upper limit for the reliability of QNLMS to the 2D spin-1/2 QHA: $0 \leq T/J < T_\Lambda/J \approx 1.0$. Meanwhile, the spin-wave velocity c_s can also be explicitly determined from Eqs. (12) and (14). For La_2CuO_4 , which is a typical 2D spin-1/2 QHA with $a = 3.79 \text{ \AA}$ and $J \approx 1500 \text{ K}$, we obtain (keeping \hbar) $\hbar c_s = 2JSa \sqrt{d + \frac{T_\Lambda}{2SJ}} \approx 0.85 \text{ eV \AA}$. This is in excellent agreement with the experimental data $\hbar c_s = 0.85 \pm 0.03 \text{ eV \AA}$ [14].

Our main results, i.e., Eqs. (12) and (14), can be further tested against the known results for the 2D QHA, among which the quantum Monte Carlo data are almost exact. Up to the three-loop correction, the QNLMS predicts [4] the asymptotic scaling behavior of the correlation length in the renormalized classical regime as

$$\xi_{3l} = A \exp(1/t) [1 - 0.5t + \mathcal{O}(t^2)], \quad (15)$$

where $A = \frac{e}{8} \frac{\tilde{c}_s}{2\pi\tilde{\rho}_s}$ is a temperature-independent prefactor, $t = \frac{T}{2\pi\tilde{\rho}_s}$ is the dimensionless temperature, and \tilde{c}_s and $\tilde{\rho}_s$ are the renormalized spin-wave velocity and spin stiffness which can be consistently determined by large- S expansion. The predicted formula ξ_{3l} is extremely sensitive to the spin stiffness and is consistent with the QMC data [15,16] at very large correlation lengths (low temperatures) for $S = 1/2$ when the best-fit value $\tilde{\rho}_s = 0.1800$ is used. However, at moderate correlation lengths, highly accurate QMC data [15] and series expansions [17] indicate a significant discrepancy which rapidly increases with S . The asymptotic scaling at the three-loop sets in at correlation lengths larger than 10^5 for $S = 1/2$ [15] and cosmological lengths for larger S .

Quite strikingly, according to the basic assumption of the large- S approach, the discrepancy between the theory and numerics, if it exists, should be significant only for small S . By contrast, in our derivation, the asymptotic scaling behavior Eq. (15) holds for arbitrary S at low temperatures, provided the effects of the intrinsic scale T_Λ are correctly taken into account. Note that the temperature dependence in Eq. (15) comes from a simple assumption that at nonzero temperature T the correlation length is much larger than the finite extent c_s/T along the Euclidean time direction in the renormalized classical regime [3,4]. In our case, the time extent is replaced by $c_s(1/T - 1/T_\Lambda)$, making the assumption more reasonable. Therefore, we only need to replace T by the rescaled temperature $\tilde{T} = \frac{TT_\Lambda}{T_\Lambda - T}$ in Eq. (15). The validity of this simple rescaling requires that $\tilde{T} < 2\pi\tilde{\rho}_s$, or $T < 0.5 \text{ J}$ for $S = 1/2$. Interestingly, the rescaling does not change the two-loop asymptotic scaling behavior. On the other hand, the shifts in c_s and g_s only modify the prefactor A but keep ρ_s unchanged. Figure 1 shows the deviations of various results from two-loop asymptotic scaling $\exp(1/t)$ as a function of t . The three-loop results of Eq. (15) in terms of t and $\tilde{t} = \frac{\tilde{T}}{2\pi\tilde{\rho}_s}$ are plotted as the 3-loop old (dashed) line

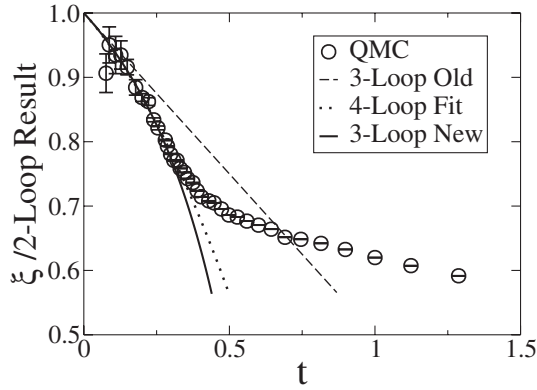


FIG. 1. Deviations of various results from two-loop asymptotic scaling as a function of t . The QMC result is obtained from Ref. [15].

and the 3-loop new (solid) line, respectively. For our three-loop result, the scaling regime begins at roughly $\xi \approx 10^2\text{--}10^3$, when $T \approx 0.3$ J. As a comparison, a suggested four-loop (dotted) line [15] is plotted by adding the correction $\mathcal{O}(t^2)$ in Eq. (15) before rescaling. The coefficient of this term is -0.75 by fitting the highly accurate QMC data which is apparently too large to be obtained within reasonable four-loop corrections [15].

Our results can also be tested against the known results for the 1D QHA. Note that in 1D, the topological term plays a crucial role, leading to the quantum critical and disordered phases for half integer and integer spins, respectively [2,18]. In the disordered phase, T_Λ can be determined by using the relation $E^2 = c_s^2 k^2 + \Delta_s^2$. This only leads to a correction $\mathcal{O}((\frac{\Delta_s}{2S})^2)$ to Eq. (14). For $S = 1/2, 1, 3/2, \text{ and } 2$, the accurate numerical results for the values of $c_s/(aJ)$ obtained by the density matrix renormalization group (DMRG) [19–21] are 1.57, 2.49, 3.87, and 4.65, respectively, which show a systematic deviation from $2S$. While, by Eq. (12), they are 1.28, 2.55, 3.84, and 5.00, respectively, providing much better predictions. The 1D QNLMSM also predicts a gap [18] in the disordered phase as $\Delta_s = Bc_s \exp(-2\pi/g_s)$, where B is a S -independent fitting parameter of order of 1. The DMRG results are $\Delta_1 = 0.411$ J for $S = 1$ [22]; $\Delta_2 = 0.085$ J for $S = 2$ [21,23]. By using the best-fitting parameter, $B \approx 2$, we find that our derivation gives $\Delta_1 = 0.438$ J and $\Delta_2 = 0.076$ J, respectively, while the large- S approach gives $\Delta_1 = 0.172$ J and $\Delta_2 = 0.015$ J, respectively. Therefore, the present 1D QNLMSM provides a better approximation for the spin-gap magnitudes in the 1D integer QHA.

In conclusion, by using a topologically invariant spin variable path integral approach, we resolve the two crucial problems in the QNLMSM description of QHA as mentioned in the beginning of this Letter. The basic parameters in the QNLMSM are unambiguously defined for arbitrary spin values. The primary tests discussed above show that the quantum fluctuations in the QHA, which are usually underestimated in the large- S approach, are now more properly

described. It should be emphasized that the construction of a low energy effective field theory from the extended phase space path integrals developed in this Letter is a general approach, in which the shortest time scale plays a crucial role for self-consistency. This approach can be applied to other generalized phase space path integrals [12] for the study of low energy physics in various strongly correlated systems.

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