Stable and metastable kinetic ferromagnetism on a ring

Ilya Ivantsov,[1] Hernan B. Xavier,[2] Alvaro Ferraz,[2] and Evgenii Kochetov[1]
[1]*Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna 141980, Russia*
[2]*Department of Experimental and Theoretical Physics, International Institute of Physics–UFRN, Natal 59078-970, Brazil*

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Performing an exact diagonalization of the effective spin problem, a ferromagnetic ground state of kinetic origin is shown to emerge in a system of N strongly correlated electrons on a L-site ring ($L > N$). A problem of N constrained spinful electrons on a L-site ring is argued to reduce to that of the spinless fermions with an effective flux threading through the ring. This phenomenon is brought about by the *quantum necklace* statistics originated by the no-double-occupancy constraint, leading to a fractional shifted electron momentum quantization. As a consequence of such special energy-level distribution, the kinetic ferromagnetism is stable only for $N = 3$. For odd $N > 3$ the fully polarized FM-state energy is only a local minimum but it is protected by a finite energy barrier that inhibits one spin-flip processes. The metastable ferromagnetic state survives perturbations of small magnitude, opening up a possibility of being experimentally observed by an appropriate tuning of interdot tunneling amplitudes in currently available quantum dot arrays.

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I. INTRODUCTION

The emergence of magnetism in itinerant electron systems presents a challenging quantum many-body physics problem. Essentially, it originates in a rather delicate quantum-mechanical balance between the potential energy saved by building strong electron correlations into the many-body wave function and a possible gain in the kinetic energy of the delocalized electrons whose hopping is inhibited by the emergent effective spin background due to correlations. A reliable description of such a phenomenon clearly requires nonperturbative approaches.

Because of this, there are only a few rigorous theoretical results for kinetic ferromagnetism (FM), with the Nagaoka FM being the most important among them [1,2]. Nagaoka's theorem predicts a FM ground state in the Hubbard model of strongly correlated electrons with a single hole (one missing electron) in the otherwise half-filled band, provided certain conditions hold (square and other bipartite lattices, infinitely strong on-site Coulomb repulsion, nearest-neighbor only coupling, and periodic boundary conditions). In this scenario a background of fully aligned electron lattice spins minimizes the total energy of a single hole. Such an effective spin background arises due to infinitely strong on-site Coulomb repulsion that strictly prohibits a double electron occupancy of the lattice sites. This is the key feature behind the Nagaoka effect. However, creating precisely one hole in a thermodynamic system is obviously an impossible constraint. There is also no consensus about the presence [3–6] or not [7,8] of the stable kinetic FM at a nonzero finite hole concentration in the thermodynamic limit or even on the role of the electron-electron interaction in this phenomenon [9]. The very fragile nature of this phenomenon does not allow generalizations of Nagaoka's theorem to a finite density of holes in the thermodynamic limit.

A natural question then arises as to whether Nagaoka's FM can really exist. The answer to this question turns out to be affirmative. Nagaoka's FM had been just a theoretical prediction since the later 1960s before it was recently experimentally observed in quantum dot arrays [10]. According to numerical calculations [11–13], three strongly correlated electrons in the 2×2 plaquette do form such FM ground state of kinetic origin. The four-dot system with three electrons has been analytically explored for many different plaquette geometries in the presence of long-range Coulomb interactions, with and without next-nearest-neighbor hopping. Specific predictions on which geometries would lead to a fully or a partially polarized FM ground state of different four-dot arrays have been thoroughly discussed [12]. However, a five-dot ring with four electrons does not exhibit a fully polarized FM ground state, despite its "Nagaoka-type" appearance (a single hole on top of a Mott insulating state with one electron per site) [12]. A general theoretical analysis is therefore warranted to explore which arrangements of electron systems on a ring would lead to a FM state and which would not. It is also important to realize under what restrictions *metastable* FM ground states could also emerge. Those issues have not been explored in the literature so far, despite the fact that that would provide more motivation for further experiments in currently available semiconductor dot-based structures in small scale systems.

Our goal in the present work is therefore twofold. First we derive the exact conditions under which the kinetic stable/metastable FM emerges on an L-site ring accommodating N electrons. Second, we discuss in what way our findings can be used in experimental setups to observe the kinetically driven FM states.

II. EXACT DIAGONALIZATION OF ONE-DIMENSIONAL RING

Nagaoka's proof implies that the so-called connectivity condition holds: Any two spin configurations can be transformed into one another by an appropriate electron hopping process. This is the case for a bipartite two-dimensional (2D) and for regular lattices of higher dimension. However it breaks down for a 1D ring. In this case Nagaoka's theorem does not apply. At first sight it may seem that the 1D solution is trivial since in a chain with open boundary conditions (BCs) the spectrum is completely degenerate with respect to its spin content. The existence of boundaries as well as the impossibility of exchanging the spin relative ordering prevents the projected electrons to access different spin configurations. Because of this the projected electrons behave essentially as spinless fermions. As a matter of fact, the Lieb-Mattis theorem tells us that in this case the ground state is realized as the lowest total spin state [14].

In contrast, for periodic BCs the situation changes drastically. The underlying configuration space is now a closed loop—a ring—with L sites and $N \leqslant L$ projected electrons. As soon as an electron crosses the boundary the corresponding spin configuration undergoes a cyclic permutation. In this way the emergent spin configurations are decomposed into disconnected parts—the quantum "necklaces"—that cannot be transformed into one another by permutations [15]. The importance of the closed loops is well known and may lead to some rather unexpected nontrivial results, such as an emergence of the kinetic antiferromagnetic order on frustrated lattices [16]. Strongly correlated electrons on a ring can be viewed as spinless particles if they are subjected to open boundary conditions. However, the periodic boundary conditions induce the presence of an effective flux produced by the quantum necklace rotation which results in the fractional shifted electron momentum quantization. It is shown that N constrained spinful electrons on a L-site ring reduces to a problem of N spinless fermions with an effective flux threading through the ring.

Our consideration is based on the strong-coupling limit of the Hubbard model—the single-band $t-J$ model of strongly correlated electrons that contains a competing kinetic energy and spin-spin exchange interaction,

$$H_{t-J} = -\sum_{ij\sigma} t_{ij}\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{j\sigma} + J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j. \tag{1}$$

Here $\tilde{c}^{\dagger}_{i\sigma} = (1-n_{i,-\sigma})c^{\dagger}_{i\sigma}$ $(\tilde{c}_{i\sigma} = (1-n_{i,-\sigma})c_{i\sigma})$ is a constrained electron creation (annihilation) operator on a site i with the spin projection $\sigma = \uparrow, \downarrow$. The electron number operator $n_{i,\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$. The symmetric matrix t_{ij} represents the hopping amplitude with $t > 0$ between the nearest neighbor sites and zero otherwise. The electron spin operator is given in terms of the Pauli matrices $\sigma_{\alpha\beta}$,

$$\mathbf{S}_i = \frac{1}{2}\sum_{\alpha\beta} c^{\dagger}_{i\alpha}\sigma_{\alpha\beta}c_{i\beta}.$$

This model captures both the antiferromagnetic ordering instability caused by the induced spin exchanges between nearly localized electrons ($\sim J$) as well as the FM itinerant magnetism due to the possible gain in the particle kinetic energy ($\sim t$).

The Nagaoka limit implies that the spin exchange interaction is dropped by setting $J = 0$. In this case and also for small-enough values of $J \ll t$ (Fig. 3) we can neglect the three-site contributions [17] which become important as soon as this condition is relaxed. The model (1) becomes exactly solvable in this limit in a 1D lattice. In this case, it exhibits a spin charge separation in the following way: The N-electron wave function of the L-site ring is decomposed as $|\psi\rangle = |\psi_r\rangle|\psi_S\rangle = |r_1, r_2, \ldots, r_N\rangle|s^z_1, s^z_2, \ldots, s^z_N\rangle$, where $r_i = 1, \ldots, L$ is the ith lattice site and $s^z_i = \pm\frac{1}{2}$ is the spin projection of the ith electron. Due to the no-double-occupancy constraint and the presence of only nearest-neighbors hopping the spin configurations are not affected by bulk hopping and they simply undergo a cyclic permutation under cross-boundary hopping. In this representation the Hamiltonian takes the form $[H_{t-J}(J=0) =: H]$:

$$H = -t\sum_{i=1}^{L-1} c^{\dagger}_i c_{i+1} - t\, c^{\dagger}_L c_1 \hat{P} + \text{H.c.}, \tag{2}$$

where c_i is the spinless fermion annihilation operator on the site i that acts only on the spatial part of wave function $|\psi_r\rangle$. The $\hat{P}$ is the cyclic spin permutation operator which affects only the spin part $|\psi_S\rangle$, with

$$\hat{P}\cdot|s^z_1, s^z_2, \ldots, s^z_N\rangle = |s^z_N, s^z_1, \ldots, s^z_{N-1}\rangle. \tag{3}$$

Since the spin part of the total wave function is affected only by the cyclic permutation operator $\hat{P}$ we can diagonalize the spin part of Hamiltonian Eq. (2) separately from its spatial part. It should be noticed that $\hat{P}$ is the block-diagonal matrix where each block corresponds to the set of configurations which can be obtained from each other by a cyclic permutation. Indeed, the $\hat{P}$ operator connects the $|\uparrow\downarrow\uparrow\downarrow\rangle$ with the $|\downarrow\uparrow\downarrow\uparrow\rangle$ but not with $|\uparrow\uparrow\downarrow\downarrow\rangle$. Thereby all the configurations connected by the cyclic permutation are inside one single spin block. The size of each block (the number of connected configurations inside the νth block) is N_ν, where ν enumerates all possible disconnected spin blocks. In general, $N_\nu = N/\phi_\nu$ where ϕ_ν is an integer depending on the symmetry of the configuration. In this way we can calculate all eigenvalues and eigenstates of $\hat{P}$:

$$\lambda_\nu(p) = e^{2\pi i p/N_\nu}$$
$$|\psi_\nu(p)\rangle = \frac{1}{\sqrt{N_\nu}}\sum_{q=0}^{N_\nu-1} e^{2\pi i p q/N_\nu}\cdot\hat{P}^q\,|\tilde{\psi}_\nu\rangle, \tag{4}$$

where $|\tilde{\psi}_\nu\rangle$ is any configuration from the νth block. The values $p = 0, \ldots, N_\nu - 1$ enumerate the eigenvalues within a given fixed νth block. Physically, the p corresponds to the spin-wave momentum induced by the cyclic permutation.

For example, a spin block with $N = N_\nu = 2$ can be thought of as that generated by the configuration $|\tilde{\psi}_\nu\rangle = |\uparrow\downarrow\rangle$. In this case Eq. (4) results in

$$|\psi_\nu(p=0)\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

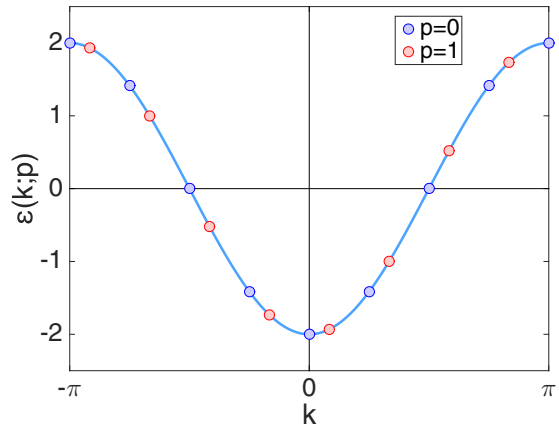

FIG. 1. Momentum quantization at various values of p for the $L = 8$ ring at $N = 3$.

and

$$|\psi_\nu(p=1)\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle),$$

which represents an even and odd under spin permutation states, respectively.

Using this basis, the Hamiltonian Eq. (2) becomes block diagonal, e.g., $H = \sum_\nu \oplus H_\nu$. The index ν together with all available values of p may be considered as the new spin quantum numbers. In each νth block we have

$$H_\nu(p) = -t\sum_{i=1}^{L-1} c_i^\dagger c_{i+1} - t\, c_L^\dagger c_1 e^{2\pi i p/N_\nu} + \text{H.c.} \qquad (5)$$

While the indexes ν and p define all possible spin configurations, $H_\nu(p)$ describes the corresponding spatial distribution of the electrons. It is essentially a tight-binding Hamiltonian of spinless fermions placed on a ring with an effective "magnetic" flux $\Phi^{(\nu)} = 2\pi p/N_\nu$ threading through the ring. Indeed, Eq. (5) implies twisted boundary conditions for fermion amplitudes, $c_i = e^{i\Phi^{(\nu)}} c_{i+L}$. By an appropriate gauge transformation, $c_i \to e^{i\Phi^{(\nu)} x_i/L} c_i$, the periodic BCs can be restored at the expense of the emergence of the Peierls phase a_{ij},

$$c_i^\dagger c_j \to c_i^\dagger c_j e^{i a_{ij}}, \quad a_{ij} = \frac{\Phi^{(\nu)}(x_j - x_i)}{L}, \quad \sum_{\text{plaquette}} a_{ij} = \Phi^{(\nu)}.$$

Note also that the solution of Eq. (5) does not depend on a specific form of the spin-wave function, but it is rather determined by the values of p.

The one-electron solution is therefore a tight-binding electron wave function,

$$|\psi(k,p)\rangle = \frac{1}{\sqrt{L}}\sum_x e^{ix\frac{2\pi}{L}\left(k+\frac{p}{N_\nu}\right)} c_x^\dagger |0\rangle$$

$$\varepsilon(k;p) = -2t\cos\left[\frac{2\pi}{L}\left(k+\frac{p}{N_\nu}\right)\right], \qquad (6)$$

with the electron momentum shifted by $2\pi p/(LN_\nu)$ (see Fig. 1). The simplest example of such a solution is a single electron wave function in the absence of correlations. In this special case, all $N_\nu = 1$ and $p = 0$ for any ν. As a result, the wave function reduces to that of a free electron as it should be.

For the many electron case the many-body wave function is the Slater determinant of the single electron wave functions with the momenta $\mathbf{k} := (k_1, k_2, \ldots, k_N)$ and with a fixed value of p which is denoted as $|\Psi_{\text{el}}(\mathbf{k}, p)\rangle$. As a result, all eigenstates and eigenvalues of Hamiltonian (2) can be written as:

$$|\Psi(\mathbf{k};\nu,p)\rangle = |\Psi_{\text{el}}(\mathbf{k},p)\rangle \cdot |\psi_\nu(p)\rangle,$$

$$E(\mathbf{k};\nu,p) = \sum_{i=1}^{N}\varepsilon(k_i;p), \qquad (7)$$

where $p = 0, \ldots, N_\nu - 1$ for each spin block ν. In this way the energy eigenvalues are determined by both the values of electron momenta $\mathbf{k}$ and the value of the spin-wave momentum p. The correlations come into play through the p/N_ν corrections to the electron momentum. This is a collective phenomena since the N_ν is proportional to a total number of electrons N. For a given spin configuration the available values of p determine the eigenenergies. For example, in the case of three electrons with the total spin $S = 3/2$ the ground-state energy is given by $E_{3/2} = -2t\{\cos(\frac{2\pi}{L}0) + \cos(\frac{2\pi}{L}1) + \cos[\frac{2\pi}{L}(-1)]\}$ while the ground-state energy corresponding to $S = 1/2$ becomes $E_{1/2} = -2t[\cos(\frac{2\pi}{L}\frac{1}{3}) + \cos(\frac{2\pi}{L}\frac{4}{3}) + \cos(\frac{2\pi}{L}\frac{-2}{3})]$. It is easy to see that $E_{3/2} < E_{1/2}$ due to the relative momentum shift by a factor of $\frac{2\pi}{L}\frac{1}{3}$.

Explicitly, these wave functions can be written in the following way: The fully polarized state $|\psi_{fp}(p)\rangle = |\uparrow\uparrow\ldots\uparrow\rangle$ is already an eigenstate of the system with the eigenvalue $\lambda_{fp} = 1$. Since cyclic permutation does not affect the configuration, we then have $N_\nu = 1$ and only the $p = 0$ condition is allowed. The state with $S = N/2$ is $N + 1$ times degenerate with respect to the different values of $S^z = -N/2, -N/2 + 1, \ldots, N/2$ and all of those states have the only one available $p = 0$ value. The energy of the fully polarized system equals the total energy produced by the free spinless fermions, as expected.

Now let us consider a spin flipped case $|\psi_{\text{sf}}\rangle = |\downarrow\uparrow\ldots\uparrow\rangle$. There are N states with $S^z = \frac{N}{2} - 1$, with $N_\nu = N$ and all of these states are connected by cyclic permutations. The corresponding eigenstates have the form:

$$|\psi_{\text{sf}}(p)\rangle = \frac{1}{\sqrt{N}}\sum_{q=0}^{N-1} e^{2\pi i p q/N}\cdot \hat{P}^q\,|\downarrow\uparrow\ldots\uparrow\rangle \qquad (8)$$

with eigenvalues $\lambda_{\text{sf}}(p) = e^{2\pi i p/N}$ and the spin-wave momentum runs over $p = 0\cdots N-1$. Here the $p = 0$ state is the $S = N/2$ state with the spin projection $S^z = N/2 - 1$ while the states with $p > 0$ correspond to the total spin $S = N/2 - 1$ and $S^z = N/2 - 1$. As a result, the fully polarized case $S = N/2$ with all possible projections S^z has the only one available $p = 0$ value for the spin-wave momentum while for the one spin flipped case $S = N/2 - 1$ the available values are $p > 0$. It is easy to see that for any value of the spin projection S^z there must be one state with $S = N/2$ and $p = 0$ and also $N - 1$ states with $S = N/2 - 1$ and $p > 0$.

Finally, for the states with $S^z \leqslant N/2 - 2$ we always have more than one disconnected spin block, which leads to further

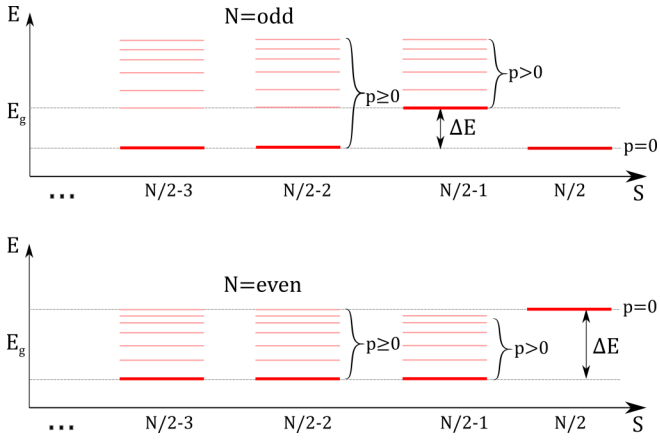

FIG. 2. The ground-state energy structure for different electron numbers N.

degeneracy of the levels. As an example, in the $S^z = N/2 - 2$ case we have $\lfloor N/2 \rfloor$ disconnected blocks and the $p = 0$ level is $\lfloor N/2 \rfloor$ fold degenerate (the symbol $\lfloor\ \rfloor$ stands for the *floor function*). While one of this degenerate levels is defined as the state with $S = N/2$ and $S^z = N/2 - 2$, all the other $\lfloor N/2 \rfloor - 1$ states correspond to $S = N/2 - 2$ total spin (the $S = N/2 - 1$ states with $p = 0$ being forbidden). As a result both the $p = 0$ and the $p > 0$ values are available for the state with $S = N/2 - 2$. Exactly the same behavior is a characteristic feature of the states with $S < N/2 - 2$.

Due to the fact that the exact eigenvalues in Eq. (7) are well known it is easy to analyze how the ground-state energy depends explicitly on p. For an even number of electrons the presence of the spin wave with the nonzero value of p produces a decrease of the eigenenergy with the minimum reached at $p = N/2$. Considering that the $p = N/2$ value is available for all values of spin except for $S = N/2$ the fully ferromagnetic state cannot be the ground state. Due to the degeneracy of the $p = N/2$ state the ground state is then a mixture of the states with a total spin $S \leqslant N/2 - 1$.

In contrast, for an odd number of electrons a nonzero value of p leads to an increase of the energy. While the minimum of the energy corresponds to $p = 0$, the next energy level corresponds to $p = 1$. As a result, the states with $S = N/2$ and $S \leqslant N/2 - 2$ have the same energy minimal value, with $p = 0$, while the state with $S = N/2 - 1$ has only the $p = 1$ level which is higher than the $p = 0$ one. That is the fully FM state with $S = N/2$ is separated from the states with $S \leqslant N/2 - 2$ by an energy barrier ΔE due to the existence of the state $S = N/2 - 1$ with higher energy (Fig. 2). A one-spin flip process implies that the system goes over into the higher energy state, which costs a certain energy. Explicitly, a value of such *a Nagaoka barrier* is

$$\Delta E = 2t \sum_{k=-(N-1)/2}^{(N-1)/2} \left\{ \cos\left(\frac{2\pi}{L}k\right) - \cos\left[\frac{2\pi}{L}\left(k + \frac{1}{N}\right)\right]\right\}. \tag{9}$$

The ground state of the odd number of electrons is thus a mixture of the FM $S = N/2$ state with the $S \leqslant N/2 - 2$ states which are not truly FM. The only one possibility to get true FM state is to put three electrons on a ring, in which case there are no longer states with $S \leqslant N/2 - 2$. The only available states are now the $S = 3/2$ and $S = 1/2$ states and

$$\Delta E = 4t \sin^2\left(\frac{\pi}{3L}\right)\left[1 + 2\cos\left(\frac{2\pi}{L}\right)\right], \tag{10}$$

with the condition that $L > 3$. Moreover, this barrier survives not only in the presence of infinity strong on-site Coulomb repulsion but also in more realistic cases including a weak-enough short-range Coulolomb repulsion, antiferromagnetic, and spin-orbit interactions, etc. [13].

In the case of an odd $N > 3$ the ground state is spin degenerate. However, realistic interactions remove this degeneracy. Since the antiferromagnetic exchange interaction has a major impact on the system compared to the other possible interactions the ground state tends to be that of the minimum spin magnitude so that the global minimum in the energy corresponds to the nonferromagnetic state. On the other hand, for weak-enough spin-spin exchange interaction the $S = N/2$ state remains separated from the $S \leqslant N/2 - 2$ states by the barrier rendering thereby the FM state a local minimum in the energy.

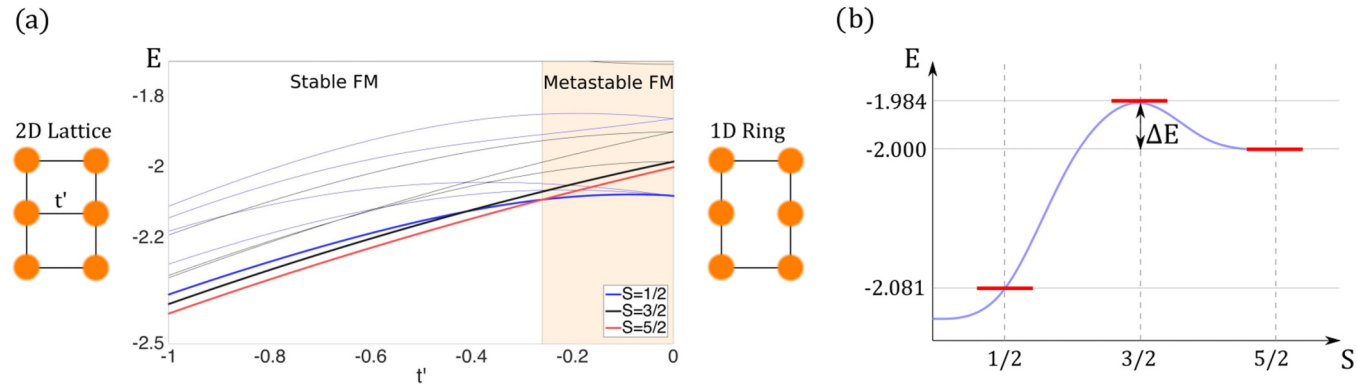

FIG. 3. (a) The transition between stable and metastable Nagaoka ferromagnetism with a change in the topology of the quantum dot array from 2D to 1D (changing the t' value). (b) The ground-states energies for the different values of total spin S for the $t - J$ model with $J = 0.05t$, $L = 6, N = 5$.

In the limit of $N \gg 1$ and $L \gg 1$, $N/L = n_e$- fixed the energy difference ΔE reduces to

$$\Delta E = \frac{2tL}{\pi} \sin(\pi n_e)\left[1 - \cos\left(\frac{2\pi}{NL}\right)\right] \approx \frac{4\pi t}{N^2 L} \sin(\pi n_e). \tag{11}$$

It is therefore clear that such Nagaoka barrier vanishes in the thermodynamic limit. Both the presence of the *disturbing* interactions and the rapid decrease of the barrier with the increasing of the ring size and the number of electrons could seem to hinder experimental observation of this phenomenon. In spite of that, it can still manifest itself in quantum dot arrays through the appearance of the *metastable* FM states.

To explicitly demonstrate how a metastable FM state can be experimentally realized, let us consider the 2×3 quantum dot array in the framework of $t - J$ model [Eq. (1)] with the large-enough value of the Coulomb repulsion corresponding to $J = 0.05$ and the hopping amplitude be t' [Fig. 3(a)] measured in units of t. Varying t' from -1 to 0 corresponds to a change in the dimension of the array from 2D cluster to 1D ring. On cooling down to a sufficiently low temperature the 2D cluster with $t' \neq 0$ displays the fully polarized FM ground state according to Nagaoka's theorem. The breaking of the t' link leads to the decrease of the $S = 1/2$ state energy relative to the $S = 3/2$ and $S = 5/2$ states. However, the $S = 5/2$ state remains with lower energy than the $S = 3/2$ one at all possible values of t' thereby protecting electrons from the spin flipping by the barrier ΔE even at a small but finite J. If the temperature is low enough, then the five-electron system remains in the metastable $S = 5/2$ state for a finite time. It should be noted that the system cooled with $t' = 0$ goes over to the global-minimum $S = 1/2$ state.

Qualitatively, the same results were obtained for the Hubbard model with the corresponding value of $U = 4t^2/J = 80t$. Such value of Coulomb repulsion is too large to be obtained in regular materials but could well be reproduced in quantum dots experiments, where the typical value of t is $t \approx 10^2$ μeV and the value of the barrier is then $\Delta E \approx 10^{-2}t \approx 1$ μeV. To observe such an effect requires that the condition $kT \ll \Delta E$ or $T \ll 10^{-2}$ K should necessarily be satisfied. The fact that modern experiments are carried out already at temperatures of the order of $T \approx 10$–100 mK allows us to suggest that experimental observation of such an effect is likely to happen soon.

III. CONCLUSION

It is shown that a problem of N constrained spinfull electrons on a L-site ring reduces to a problem of spinless electrons with an effective flux threading through the ring. The flux arises due to the nonconnectivity of the emergent spin configurations. It gives rise to the fractional shifted electron momentum quantization induced by the cyclic permutations group. Nagaoka's ferromagnetism sets in only in the case in which there are three electrons on the ring with $L > 3$. For an odd number of electrons greater than three the FM state can only be realized as a local energy minimum state protected by a corresponding Nagaoka barrier. As a result, the fully polarized state for $N > 3$ is truly a metastable state. The progress in quantum dots fabrication provides a real possibility to observe such metastable ferromagnetism experimentally. Specifically, we present experimental signatures of the metastable FM using a quantum dot device to host a 2×3 lattice of electrons. Effectively tuning the geometry of the system from a 2D cluster to a 1D ring automatically drives the system into the metastable ground state.

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