Power-law spin correlations in a perturbed honeycomb spin model

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We consider spin-$\frac{1}{2}$ model on the honeycomb lattice $[1]$ in presence of a weak magnetic field $h_a \ll 1$. Such a perturbation destroys exact integrability of the model in terms of gapless fermions and static $Z_2$ fluxes. We show that it results in appearance of a long-range tail in the irreducible dynamic spin correlation function: $\langle s^z(t,r)s^z(0) \rangle \propto h_a^2 f(t,r)$, where $f(t,r) \propto [\max(t,r)]^{-4}$ is proportional to the density polarization function of fermions.

Quantum spin liquids, QSL’s (see e.g. Refs. [2–5]) present examples of strongly correlated quantum phases which do not develop any kind of local order, while their specific entropy vanishes at zero temperature. Critical, or algebraic QSL’s are characterized by spin correlation functions that decay as some power of distance and time. In some cases, the correlation asymptotics can be deduced from a representation of spin operators in terms of almost-free fermions [4]. However, a complete calculation based on a microscopic Hamiltonian has not been demonstrated due to the lack of suitable exactly solvable models (in more than one spatial dimension). We show in the present Letter that the anisotropic spin-$\frac{1}{2}$ model on the honeycomb lattice, proposed by one of us [1], can be used as a starting point for the construction of an analytically treatable critical QSL. This result may seem surprising since it is known [2] that the original model [1] possesses no spin correlations at the distances longer than a single lattice bond. We will see however, that a small perturbation of the model [1], e.g. weak external magnetic field, is sufficient to ”turn on” long-range spin correlations, albeit with a small overall prefactor. Thus we disagree with the statement made in Ref. [7] that short-range character of spin correlations survives in the presence of a weak magnetic field.

We consider the model defined by the Hamiltonian:

$$\mathcal{H} = J \sum_{ij} (\sigma_i n_i) (\sigma_j n_j) - \sum_i h_i \sigma_i.$$  \hspace{1cm} (1)

Unit vectors $n_i$ are parallel to $x$, $y$ and $z$ axis for the corresponding links $x$, $y$ and $z$ of the honeycomb lattice, see Fig.1. At $h_i = 0$ the Hamiltonian [1] was solved exactly [1] via a mapping to a free fermion Hamiltonian. In this approach, each spin $\sigma_i$ is represented in terms of four Majorana operators $c_i$, $c_i^\dagger$, $c_i^\gamma$, $c_i^\gamma^\dagger$ with the following anticommutation relations: $\{c_i^\alpha, c_j^\beta\} = 2 \delta_{ij} \delta_{\alpha\beta}$, so that $\sigma_i^\alpha = ic_i^\alpha c_i^\gamma$. In terms of these new operators, the zero-field Hamiltonian reads $\mathcal{H} = -iJ \sum_{ij} c_i u_{ij} c_j^\dagger$ and $u_{ij} = i c_i^\gamma c_j^\gamma$ are constants of motion: $[\mathcal{H}, u_{ij}] = 0$, with $u_{ij} = \pm 1$. The ground state $|G\rangle$ corresponds to an arbitrary choice of $\{u_{ij}\}$ that minimizes the energy. It is convenient to introduce the notion of $Z_2$ flux, defined for each hexagon $\pi$ as a product $\phi_\pi = \prod_{ij} u_{ij}$ (since $u_{ij} = -u_{ji}$, we have to choose a particular ordering in this definition: $i$ is even sublattice, $j$ is odd sublattice).

The ground state of this model is a symmetrized sum of states with different sets of integrals of motion $\{u_{ij}\}$, corresponding to all fluxes equal to 1. For practical calculations of physical quantities, one does not have to implement such symmetrization and can assume that all $u_{ij} \equiv 1$. We denote by $H$ the corresponding Majorana Hamiltonian: $H = -iJ \sum_{ij} c_i^\dagger c_j$. It can be diagonalized with the use of Fourier transformation. The spectrum of the resulting free fermions is gapless and has two conic points. To begin, we recall the calculation of the spin-spin correlation function $g^\alpha_{ij}(t) = \langle \sigma_i^\alpha(t)\sigma_j^\beta(0) \rangle$ in the unperturbed model with $h = 0$. Spin operator $\sigma_i^\alpha$ acting on the ground state produces two $Z_2$ fluxes and creates a fermion. Since states with different flux configurations are mutually orthogonal and fluxes do not move in the process of time evolution governed by the Hamiltonian $\mathcal{H}$, a non-zero result for the correlation function is possible only if the second spin operator $\sigma_j^\beta$ creates the same pair of fluxes. Thus the sites $i$ and $j$ are either the same or nearest neighbors. For larger separations between $i$ and $j$, one has $g_{ij} = 0$. However, this result is due to the static nature of $Z_2$ fluxes; furthermore, the ground

FIG. 1: A honeycomb lattice fragment with the $z$–$z$ link that belongs to a given elementary cell. The indicated vector $q_+^\alpha = \hat{a}$ shows the direction of oscillations found in the $\langle s^z(0)s^z(r) \rangle$ correlation function.
state is a linear combination of states with the same flux pattern. Both these features are destroyed by any perturbation (for example, external magnetic field) that does not commute with operators \( \{ u_{ij} \} \).

In this paper, we consider the honeycomb lattice model with an external magnetic field, which is treated as a weak perturbation. Before delving into calculations, we note that a generic magnetic field opens a gap \( \Delta \) in the fermionic spectrum \([1]\), with \( \Delta \sim h_xh_yh_z/J^2 \). In what follows we neglect this gap. This is definitely possible if one of the field components vanishes, i.e., if the field is directed in one of the coordinate planes. For the generic field direction, our results for spin correlations are applicable for intermediate distances, \( 1 \ll r \ll 1/\Delta \).

For simplicity we discuss the total spin in the \( r \)-th elementary cell, \( s_r = \sigma_{r,1} + \sigma_{r,2} \) and calculate \( z-z \) correlations only. Since the external magnetic field induces finite magnetization, \( \langle s_z^2 \rangle \neq 0 \), we study the irreducible correlation function: \( g(t,r) = \langle (s_z^2(t)s_0^2(0)) \rangle \). We are interested in the long-time and/or long-distance asymptotics of \( g(t,r) \).

It is convenient to introduce complex bond fermions, defined as follows: \( \psi_r = \frac{1}{2}(\epsilon_r, 1 + i \epsilon_r) \) and \( \phi_r = \frac{1}{2}(\epsilon_r, 1 + i \epsilon_r) \). Operator \( \phi_r \) creates two fluxes in the plaquettes adjacent to the \( z \)-link in the elementary cell \( r \). Note, that \( \phi_r^+ \phi_r = \frac{1}{2} \delta_{r,r} \), and hence the ground-state wave function \( |G \rangle \) satisfies \( \phi_r^+ \phi_r |G \rangle = |G \rangle \). Spin operator factorizes in the following way: \( s_z^2 = 2i \psi_r^\dagger \psi_r \psi_r^\dagger \psi_r \), where vectors \( \psi_r^\dagger = (\psi_r, \psi_r^\dagger) \), \( \phi_r^\dagger = (\phi_r, \phi_r^\dagger) \) are introduced and summation over \( \alpha \) is implied. In the absence of magnetic field, the correlation function of flux operators \( \psi_r \) is local: \( G_\phi(r,t) = \langle \phi_{r}^\dagger(t)\phi_{0}(0) \rangle = \varphi(t) \delta_{r,0} \), which leads to locality of the spin correlations. However, once the magnetic field is turned on, one finds \( G_\phi(r,t) \) to be non-zero and proportional to \( h_z^2 \) at any \( r \), which leads to spin correlation at large distances. We start from the expression for \( \langle s_z^2(t)s_0^2(0) \rangle \), expanded up to the second order in \( h_z \):

\[
\langle s_z^2(t)s_0^2(0) \rangle = -\frac{h_z^2}{2} \sum_{r_1,r_2} \int_0^\infty d\tau_1 d\tau_2 \cdot \langle T s_z^2(t) s_0^2(0) s_{r_1}^z(\tau_1) s_{r_2}^z(\tau_2) \rangle.
\]

The irreducible correlation function equals \( g(t,r) = \langle s_z^2(t)s_0^2(0) \rangle - \langle s_0^2(0) \rangle^2 \), where

\[
\langle s_0^2(0) \rangle = -i h_z \sum_r \int d\tau \langle T s_0^2(0) s_z^z(\tau) \rangle.
\]

Thus we have to calculate two-spin and four-spin correlation functions. For these correlation functions to be non-zero, the flux configuration which results from the action of the two (four) spin operators on the ground state should coincide with the original flux configuration. In particular, the two-spin correlator vanishes unless \( r = 0 \), so that we have \( \langle T s_0^2(0) s_z^z(\tau) \rangle = u(\tau) \delta_{r,0} \) with \( u(\tau) = \langle T s_0^2(0) s_0^2(\tau) \rangle \). It is clear that \( u(-\tau) = u(\tau) \).

The expression for the magnetization thus simplifies:

\[
\langle s_z^2 \rangle = -2i h_z \int_0^\infty u(\tau) d\tau.
\]

Similarly,

\[
\langle T s_z^2(t) s_0^2(0) s_{r_1}^z(\tau_1) s_{r_2}^z(\tau_2) \rangle = f_1(r,t,\tau_1,\tau_2) \delta_{r_1,0} \delta_{r_2,0} + f_2(r,t,\tau_1,\tau_2) \delta_{r_1,0} \delta_{r_2,r},
\]

where

\[
f_1(r,t,\tau_1,\tau_2) = \langle T s_z^2(t) s_0^2(0) s_{r_1}^z(\tau_1) s_0^2(\tau_2) \rangle, \quad (5)
\]

\[
f_2(r,t,\tau_1,\tau_2) = \langle T s_z^2(t) s_0^2(0) s_{r_1}^z(\tau_1) s_r^z(\tau_2) \rangle.
\]

In the \( t \to \infty \) limit, the leading contributions to \( f_1 \) and \( f_2 \) come from the regions \( \tau_1 \approx t, \tau_2 \approx 0 \) and \( \tau_1 \approx 0, \tau_2 \approx t \), respectively. We will see that the product of spin operators at nearby times, e.g. \( s_z^2(t)s_z^2(\tau_2) \) in the second case, reduces to the product of two fermion operators (up to some renormalization). It follows that the four-spin correlation function is asymptotically proportional to the density polarization function of free fermions.

Note that the Wick theorem is not directly applicable to spin averages because each spin operator creates both a fermion and some flux, the latter acting as a scattering potential for propagating fermions. To proceed with the calculation, one has to rewrite spin operators \( s_z^2 \) in equations (5) in terms of fermions \( \psi \) and \( \phi \), and then move the \( \phi \) operators to the right, commuting them with exponential evolution factors. To this end, we use the identities

\[
\phi_r e^{iH_\tau} = e^{iH_\tau} \phi_r, \quad \phi_r^\dagger e^{iH_\tau} = e^{iH_\tau} \phi_r^\dagger, \quad (6)
\]

where the Hamiltonian \( H_\tau \) differs from the original Hamiltonian \( H \) by inverting sign of the \( u \) variable which belongs to the \( z \)-link in the elementary cell \( r \): \( H_\tau = H + V_\tau \), where \( V_\tau = 4J (\psi_r^\dagger \psi_r - \frac{1}{2}) \). In this way, all spin correlators can be represented as correlators of non-interacting fermions in the presence of external time-dependent potential. The calculation of \( u(\tau) \) is a simple task discussed in Refs. [2,8]. Using the identity \( e^{iH_\tau}e^{-iH_\tau} = T \exp \left( -i \int_0^\tau V_\tau(\tau) d\tau \right) \), one arrives at the following result:

\[
u(\tau) = 4 \left( T \psi_0(\tau) \bar{\psi}_0^\dagger(0) e^{-i \int_0^\tau V_\tau(\tau) d\tau} \right) \quad \text{for} \quad \tau > 0.
\]

The next step is to calculate \( f_{1,2}(r,t,\tau_1,\tau_2) \). We consider explicitly all different time orderings in the expression (5); it is enough to choose \( t > 0 \), since \( g_r(-t) = g_{-r}(t) \):

1) \( \tau_2 > \tau_1 > t > 0 \);
2) \( \tau_2 > t > 0 > \tau_1 \);
3) \( t > 0 > \tau_2 > \tau_1 \);
4) \( t > \tau_2 > \tau_1 > 0 \);
5) \( t > \tau_2 > 0 > \tau_1 \);
6) \( \tau_2 > t > \tau_1 > 0 \),
while other 6 domains $1^{'..6'}$ can be obtained by the permutation $\tau_1 \leftrightarrow \tau_2$.

Let us illustrate how to perform the calculation of $f^{(j)}_{1,2}$

\[
\begin{align*}
f^{(2)}_1 &= \langle s_0^+(\tau_2) s_0^-(t) s_0^-(0) s_0^+(\tau_1) \rangle = 16 \left\langle e^{iH_{\tau_2} \phi_0^+} e^{-iH_{\tau_2} \phi_{\tau_2}^+} e^{iH_t \phi_{\tau_1}^+} e^{-iH_t \phi_{\tau_1}^+} e^{-iH_{\tau_1} \phi_{\tau_1}^+} e^{iH_{\tau_1} \phi_{\tau_1}^+} e^{-iH_{\tau_1} \phi_{\tau_1}^+} \right\rangle = \\
&= 16 \left\langle e^{iH_{\tau_2} \phi_0^+} e^{-iH_{\tau_2} \phi_{\tau_2}^+} e^{iH_0 \phi_{\tau\cdot t}} e^{-iH_0 \phi_{\tau\cdot t}} e^{iH_{\tau_1} \phi_{\tau_1}^+} e^{-iH_{\tau_1} \phi_{\tau_1}^+} \right\rangle = \\
&= -16 \left\langle T\psi_0(\tau_2) \psi_0(t) \psi_0^+(0) \psi_0^+(\tau_1) e^{-i \int V^{(2)}(\tau) d\tau} \right\rangle. \\
\end{align*}
\]

To proceed from the first to the second line, we used the fact that the only relevant sequence of superscripts is $\alpha\beta\gamma\delta = 1122$ (recall that $\phi_{\beta\gamma}^+ \phi_{\delta}^+ |G\rangle = |G\rangle$, while $\phi_{\beta\gamma}^+ \phi_{\delta}^+ |G\rangle = 0$ and $\phi_{\beta\gamma}^+ = \phi_{\tau\cdot t}^2 = 0$). Similarly, for $f^{(2)}_2$ one obtains:

\[
f^{(2)}_2 = 16 \left\langle T\psi_r(\tau_2) \psi_r^+(t) \psi_0^+(0) \psi_0^+(\tau_1) e^{-i \int V^{(2)}(\tau) d\tau} \right\rangle.
\]

The potentials $V^{(2)}_{1,2}(\tau)$ are piece-wise-constant functions of time which can be easily read off the order of fermionic operators in [7, 8]:

| $V^{(2)}_{1,2}(\tau)$ | $(-\infty; \tau_1)$ | $(\tau_1; 0)$ | $(0; t)$ | $(t; \tau_2)$ | $(\tau_2; \infty)$ |
|----------------------|-------------------|--------------|-------------|----------------|------------------|
| $V^{(2)}_1(\tau)$   | $0$               | $V_r$        | $V_r + V_0$| $V_0$          | $0$              |
| $V^{(2)}_2(\tau)$   | $0$               | $0$          | $V_r$      | $V_0$          | $0$              |

In the same way exact expressions for $f^{(j)}$ are analogous to [4], can be obtained for all other time domains $1...6$. However, they can hardly be evaluated exactly in the closed form. The problem of their calculation resembles the one encountered while exploring the Fermi Edge Singularity problem [10], so we can analyze it similarly.

The representation of spin correlation functions in the form [9] allows us to use the Wick theorem for fermions, which makes a diagrammatic expansion of $f^{(j)}_i$ over the potential $V^{(j)}_i$ possible. Note that apart from the normal Green function $G(t, r) = \langle T\psi_r(t, \psi_0^+(0, 0) \rangle$, the anomalous Green function $F(t, r) = \langle T\psi_r(t, \psi_0(0, 0) \rangle = \langle T\psi_0^+(0, 0) \psi_0^+(t, r) \rangle$ has also to be taken into account (we calculate both of them below). The sum of all diagrams for each of $f^{(j)}_i$ is of the form $f^{(j)}_i = 16 e^{C^{(j)}_i} L^{(j)}$, where the first factor is the the sum of closed-loop diagrams, and the second factor $L^{(j)}_i$ is the a sum of open-line diagrams.

The closed-loop contribution equals $e^{C^{(j)}_i(t, \tau_1, \tau_2)} = \langle T e^{-i \int V^{(j)}(\tau) d\tau} \rangle$. In the limit of large time separation between pairs of points $\{t, \tau_1\}$, $\{0, \tau_2\}$ or $\{t, \tau_2\}$, $\{0, \tau_1\}$, the asymptotic form of $C^{(j)}_i$ can be simply determined.

For the particular time domain $j = 2$. We get for $L^{(2)}_1$ the following expression (summation over $\alpha...\delta$ is implied):

\[
\begin{align*}
C^{(2)}_1 &\approx -i \left( \Omega (t + \tau_2 - \tau_1) + \delta \Omega t \right), \\
C^{(2)}_2 &\approx -i \Omega (\tau_2 - \tau_1 - t). \\
\end{align*}
\]

In this equation, $\Omega$ is the energy of the fermionic ground state in the presence of two adjacent fluxes ($\Omega \approx 0.04 J$, see [1]), while $\delta \Omega_t$ stands for the interaction energy of two flux pairs separated by distance $r$. Therefore, the factor $\exp \left( C^{(j)}_i(t, \tau_1, \tau_2) \right)$ rapidly oscillates with frequency $\Omega$.

Each term in the sum of open-line diagrams corresponds to a particular pairing of four fermionic operators in the product [7] or [8]. For example, $L^{(2)}_2$ is given by the following equation:

\[
L^{(2)}_2 = \langle T\psi_r(\tau_2) \psi_r^+(t) \psi_0^+(0) \psi_0^+(\tau_1) \rangle \int V^{(2)}(\tau) d\tau - \langle T\psi_r(\tau_2) \psi_0^+(0) \psi_0^+(\tau_1) \rangle - \langle T\psi_r(\tau_2) \psi_0^+(\tau_1) \rangle \int V^{(2)}(\tau) d\tau ,
\]
a small neighborhood of the boundary points due to oscillations of the integrand, so the corresponding expression in \( \mathbf{3} \) is of the form of fermionic density-density correlation function. Now we have to calculate \( L_{(2)}^2 \) for \( \tau_1 \approx 0 \) and \( \tau_2 \approx t \). Note that for such time arguments, the external potential \( V_{(2)}^\perp \) as a function of \( \tau \) turns on for two short intervals (of the order of \( \Omega^{-1} \)), while the separation between the pulses is large, \( t \gg J^{-1} \). In this case the long-time (or large-distance) asymptotics of the correlation function reads \( \langle T \psi_\tau \langle \psi_\tau \rangle \rangle \approx G_0(t) \phi(0 - \tau_1) \bar{\phi}(\tau_2 - t) \), where \( \phi(\tau), \bar{\phi}(\tau) \) are some dimensionless functions of \( J \tau \). The double integral in \( \mathbf{10} \) is thus factorized, and the renormalization due to the functions \( \phi(\tau), \bar{\phi}(\tau) \) adds an overall numerical coefficient only, which we denote by \( \h_0^{-2} \) (it is the same for the contributions from all time domains). Calculating the dominant first term in \( \mathbf{10} \) (the other oscillations as functions of \( t \)), we obtain \( g_2^{(2)} \):

\[
g_2^{(2)} = -16h_x^2 \left( \int_0^\infty u(\tau) d\tau \right)^2 - 16h_x^2 h_0^2 \left( F(t, r) F(-t, -r) + G(t, r) G(-t, -r) \right).\]

Similar considerations are applicable for the other time domains. 1..6 show that all relevant contributions have a similar feature: the integration over \( \{\tau_1, \tau_2\} \) is dominated by some neighborhood of points 0 and \( t \). Collecting everything and subtracting \( s_0^2(0)^2 \), we obtain:

\[
g(t, r) = -64\frac{h_x^2}{h_0^2} \left( F(t, r) F(-t, -r) + G(t, r) G(-t, -r) \right) \]

where free fermion Green functions \( G \) and \( F \) are calculated below in Eq. 12. Thus we have found that the spin correlation function \( g(t, r) \) is proportional to the density-density correlation function of band fermions, with the coefficient \( \approx h_x^2 \). The parameter \( h_0 \) in Eq. 11 can be estimated (up to a numerical constant) to be \( h_0 \sim J \).

Now we turn to the calculation of fermionic Green functions \( G(t, r) \) and \( F(t, r) \) which enter Eq. 11. The expression for "vector" composed of these Green functions in the energy-coordinate representation reads:

\[
(G_x(r), F_x(r)) = \frac{2i}{N} \sum \frac{(e^{i\lambda f_p} \cos(|\mathbf{p}|) - i\mathbf{R} f_p \sin(|\mathbf{p}|))}{c^2 - |\mathbf{p}|^2 + i\delta}.
\]

where \( f(\mathbf{p}) = 2iJ(1 + e^{2\pi\mathbf{n}_1} + e^{2\pi\mathbf{n}_2}) \) and \( \mathbf{n}_{1,2} = (\pm \frac{\sqrt{3}}{2}, \frac{\sqrt{3}}{2}) \) in the standard \((x, y)\) coordinates. We expand \( f(\mathbf{p}) \) near the conical point \( \mathbf{K} = \left( \frac{2\pi}{3}, \frac{2\pi}{3}, \frac{2\pi}{3} \right) \) to get long-time behavior of \( G(t, r) \) and \( F(t, r) \). Substituting these asymptotics to Eq. 11, we obtain the final result:

\[
g(t, r) = \frac{16}{\pi^2} \left[ \frac{h_x}{h_0} \right]^2 \left( \frac{r^2 - 3(2\pi \mathbf{q}_z^\perp - \mathbf{r})^2}{r^2 - 3(2\pi \mathbf{q}_z^\perp - \mathbf{r})^2} \right),
\]

where \( \mathbf{q}_z^\perp = \mathbf{x} \) is the unit vector along \( x \), orthogonal to the direction of \( z-z \) link. The singularity of this expression at \( r/t = \sqrt{3}J \) is cut off by the finite width of the Brillouin zone, which was sent to infinity while calculating integrals leading to Eqs. 13. The above result may seem surprising due to the apparent anisotropy demonstrated by fast oscillations in expression 13 as a function of the \( x \)-component of \( \mathbf{r} \). This anisotropy is due to our choice to calculate correlations of the \( z \) components of the spin in the unit cell. Similar calculation for \( x \) or \( y \) components lead to analogous results with anisotropy vectors \( \mathbf{q}_x^\perp, \mathbf{q}_y^\perp \), which are perpendicular to the corresponding lattice links. The correlation function 13 was calculated in the lowest nontrivial order over perturbation \( h_x \). To account for higher-order terms in this expansion, one should study the effects of flux motion upon the fermion polarization function.

In conclusions, we have shown that under weak perturbation due to magnetic field, spin operators acquire nonzero projection \( \sim h_x^2 \) on the density of band fermions, thus long-range spin correlations appear. Therefore weakly perturbed honeycomb spin model may be considered as an example of the critical QSL. We expect that the same mechanism of the coupling of spins to fermion density can be realized for similar models on the decorated honeycomb lattice. 3.5. For the gapful state 3, we expect spin correlations to decay with a correlation length/time determined by the gap in the fermion spectrum, whereas for the spin metal state 3 the asymptotic behavior \( f(t, r) \propto [\max(t, r)]^{-1} \) is expected. Another perturbation leading to the similar effect is a weak modification of the triad of \( \mathbf{n} \) vectors, which will also produce nonzero spin correlations at arbitrary distances.

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