Long-range spin correlations in a honeycomb spin model with magnetic field

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We consider spin-1/2 model on the honeycomb lattice (Ann. Phys. **321**, 2 (2006)) in presence of weak magnetic field $h_\alpha \ll J$. Such a perturbation treated in the lowest nonvanishing order over h_α leads (Phys. Rev. Lett. **106**, 067203 (2011)) to a power-law decay of irreducible spin correlations $\langle\langle s^z(t,r)s^z(0,0)\rangle\rangle \propto h_z^2 f(t,r)$, where $f(t,r) \propto [\max(t, Jr)]^{-4}$. In the present Letter we studied the effects of the next order of perturbation in h_z and found an additional term of the order h_z^4 in the correlation function $\langle\langle s^z(t,r)s^z(0,0)\rangle\rangle$ which scales as $h_z^4 \cos\gamma/r^3$ at $Jt \ll r$, where γ is the polar angle in the 2D plane. We demonstrate that such a contribution can be understood as a result of a perturbation of the effective Majorana Hamiltonian by weak imaginary vector potential $A_x \propto ih_z^2$.

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Introduction. Quantum spin liquids, QSL's (see e.g. Refs. [1–5]) 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. One exactly solvable case of the critical QSL is presented by the celebrated Kitaev honeycomb spin model [6], for a more recent review see Ref. [7]. Although long-range spin correlations exactly vanish in this model, it presents convenient starting point for the construction of controllable theories possessing long-range spin correlations, since the spectrum of the model contains gapless fermions. Honeycomb model [6] was originally invented as a simplest solvable spin model possessing nontrivial topological phases, relevant in the context of topological quantum computing; later it has been found that similar spin interactions can be realized in the honeycomb-lattice oxides Na_2IrO_3 and Li_2IrO_3 [8–10]. In a realistic situation, low-energy effective description of these materials is given by a mixture of the Kitaev and Heisenberg interactions with weights depending on the microscopic parameters. Alternatively, Heisenberg–Kitaev (HK) model appears as a low-energy theory of a Hubbard model defined on a honeycomb lattice with spin-dependent hopping [11]. Interestingly enough, exact diagonalization and a complementary spin-wave analysis [12] show that spin-liquid phase near the Kitaev limit is stable with respect to small admixture of Heisenberg interactions [13].

However, Kitaev model in its original form does not possesses long-range spin correlations, moreover, its spin correlators are strictly local [14]. A perturbative addition of the Heisenberg interaction does not lead to a power-law spin correlations [15]. In order to produce a spin-liquid phase with long-range correlations, some other terms should be added to the effective Hamiltonian. In particular, such a terms appear naturally if HK Hamiltonian is obtained as a low-energy limit for the Hubbard Model [11]. Another perturbation which does not destroy spin-liquid phase but renders correlations non-local is magnetic field [16, 17].

Importantly, the case of a weak magnetic field $h_z\sigma_i^z$ added to the Kitaev model is tractable analytically and in the paper [16] it was shown that indeed algebraic QSL can be obtained as a result of such a simple perturbation applied to the Kitaev model. It was found [16] that it leads to an appearance of long-range (power-law) contribution to the irreducible spin-spin correlation function $S(\mathbf{r},t) = \langle\langle s_r^z(t)s_0^z(0)\rangle\rangle$, where $s_r = \sigma_{r,1} + \sigma_{r,2}$ is the total spin of an elementary cell. This result was obtained in the leading non-vanishing order in the perturbation strength: power-law contribution to $S(\mathbf{r},t)$ is proportional to h_z^2. Qualitatively, the result of Ref. [16] can be interpreted in very simple terms: magnetic field provides a coupling between the spin operator and the operator of density of Majorana fermions which are used to diagonalize the unperturbed ($h_z = 0$) Hamiltonian (see below). Once this coupling was demonstrated, the rest

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of the calculation is rather straightforward: one should calculate density-density correlation function for these free fermions.

However, it worked this way in the lowest order in h_z only. Should one be interested in the effects of higher order in the magnetic field, its influence upon the properties of Majorana fermions should be studied. This is the subject of the present Letter: we demonstrate how to calculate spin-spin correlation function in the next (h_z^4) order and then show that the result can be understood in a very simple terms of rather natural perturbation applied to the free Majorana problem.

We consider the model defined by the Hamiltonian:

$$\mathcal{H} = J \sum_{l=\langle ij \rangle} (\sigma_i \mathbf{n}_l)(\sigma_j \mathbf{n}_l) - \sum_i \mathbf{h}_i \sigma_i. \tag{1}$$

Unit vectors $\mathbf{n}_l$ are parallel to x-, y-, and z-axis for the corresponding links x, y, and z of the honeycomb lattice: $\mathbf{r} = m_1\mathbf{n}_1 + m_2\mathbf{n}_2$ with integer $m_{1,2}$ and translation vectors $\mathbf{n}_{1,2} = (\pm\frac{1}{2}, \frac{\sqrt{3}}{2})$. At $\mathbf{h}_i \equiv 0$ the Hamiltonian (1) was solved exactly [6] via a mapping to a free fermion Hamiltonian. In this approach, each spin σ_i is represented in terms of four Majorana operators c_i, c_i^x, c_i^y, c_i^z with the following anticommutation relations: $\{c_i^\alpha, c_j^\beta\} = 2\delta_{ij}\delta_{\alpha\beta}$, so that $\sigma_i^\alpha = ic_ic_i^\alpha$. In terms of these new operators, the zero-field Hamiltonian reads $\mathcal{H} = -iJ\sum_{\langle ij\rangle} c_i u_{ij} c_j$ and $u_{ij} = ic_i^\alpha c_j^\alpha$ are constants of motion: $[\mathcal{H}, u_{ij}] = 0$, with $u_{ij} = \pm 1$. The ground state $|G\rangle$ corresponds to a choice of $\{u_{ij}\}$ that minimizes the fermionic energy. It is convenient to introduce the notion of Z_2 flux, defined for each hexagon π as a product $\phi_\pi = \prod u_{ij}$ (since $u_{ij} = -u_{ji}$, we have to choose a particular ordering in this definition: $i \in$ even sublattice, $j \in$ 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. Such a symmetrization, however, never needs to be implemented in practice and $S(\mathbf{r}, t)$ can be computed with unprojected eigenstates. This is possible due to gauge invariance of the spin operators (in general, one should take care of the parity of fermions in the physical sector, which can depend on the boundary conditions [18]).

Fixing the gauge (all $u_{ij} \equiv 1$), we denote by H the corresponding Majorana Hamiltonian: $H = -iJ\sum_{\langle ij\rangle} c_i c_j$. It can be diagonalized with the use of Fourier transformation; as a result the spectrum of unperturbed Kitaev model reads $\epsilon(p) = \pm|f(\mathbf{p})|$ where $f(\mathbf{p}) = 2iJ(1 + e^{i(\mathbf{p},\mathbf{n}_1)} + e^{i(\mathbf{p},\mathbf{n}_2)})$. It is gapless and has two conic points (lattice constant is set to be unity):

$$\mathbf{K}_{1,2} = \left(\pm\frac{2\pi}{3}, \frac{2\pi}{\sqrt{3}}\right). \tag{2}$$

Long-range correlation functions are determined by the fermionic fields with momenta close to either $\mathbf{K}_1$ or $\mathbf{K}_2$. Our original site fermions $c_{i\lambda}$ are real (here i enumerates elementary cells while $\lambda = 1, 2$ selects one of the two sublattices), and after Fourrier transform we have $c_\lambda^+(\mathbf{q}) = c_\lambda(-\mathbf{q})$. As long as we are interested in low-energy behavior, it is possible to work with complex fermionic fields $a_\lambda(\mathbf{p})$ and $a_\lambda^+(\mathbf{p})$ with small momentum $\mathbf{p}$ defined as follows:

$$\begin{aligned} a_\lambda(\mathbf{p}) &= c_\lambda(\mathbf{K}_1 + \mathbf{p}), \\ a_\lambda^+(\mathbf{p}) &= c_\lambda(\mathbf{K}_2 - \mathbf{p}). \end{aligned} \tag{3}$$

In terms of $a_\lambda(\mathbf{p})$ fermions our problem can be formulated in a continuous form, without reference to the underlying lattice. Now we introduce 2×2 Pauli matrices $\sigma_{\lambda\mu}^\alpha$, acting in the sublattice space, with $\alpha = x$ or y, and present our low-energy Hamiltonian in the Dirac form

$$H_F = \sqrt{3}J\sum_{\mathbf{p}} \bar{a}_\lambda(\mathbf{p})\sigma_{\lambda\mu}^\alpha p^\alpha a_\mu(\mathbf{p}), \tag{4}$$

where new "Dirac-conjugated" fields $\bar{a}_\lambda(\mathbf{p}) = -ia_\nu^+(\mathbf{p})\sigma_{\nu\lambda}^z$ are introduced for convenience (matrix $-i\sigma^z$ is acting like charge conjugation operator).

We have shown in the previous paper [16], that magnetic field induces the coupling of spin to Fermionic density, leading to the following result:

$$S^{(2)}(\mathbf{r}, t) = \frac{4}{\pi^2}\left(\frac{h_z}{h_0}\right)^2 \times \\ \times \frac{3J^2t^2\left(Z_1^2 + Z_2^2\right) - r^2\left(Z_1^2 + Z_2^2 - 2Z_1Z_2\cos 2\gamma\right)}{\left(3J^2t^2 - r^2\right)^3}, \tag{5}$$

where $h_0 \sim J$ and we have introduced $Z_{1,2} = e^{i\mathbf{K}_{1,2}\mathbf{r}}$, where conical points wave vectors $\mathbf{K}_{1,2}$ are defined in Eq. (2) and γ stays for the polar angle of $\mathbf{r}$ in the (x, y). Equivalent form of (5) is

$$S^{(2)}(\mathbf{r}, t) = \\ = \frac{8}{\pi^2}\left(\frac{h_z}{h_0}\right)^2\left[\frac{3J^2t^2 + r^2\cos 2\gamma}{(3J^2t^2 - r^2)^3} + \frac{\cos 2\pi m/3}{(3J^2t^2 - r^2)^2}\right] \tag{6}$$

with $m = m_1 - m_2$.

Below we will employ the same method of calculation, used in Ref. [16] to obtain Eq. (5), generalizing it to a next order in magnetic field. We will be interested in long-time asymptotics of the spin-spin correlation function, hence rich and important physics of Fermi-edge-like singularity for Majorana Fermions [19, 20] will be of limited importance for us; these time-dependents effects will only restrict the relevant domain of the integration over the intermediate states in the corresponding perturbation theory, as described below.

Reduction of the spin-spin correlation function to the fermionic one. We start from the expression for the spin-spin correlation function $S(\mathbf{r},t)$, expanded up to the fourth order in magnetic field h_z. It reads (compare with Eq. (2) in Ref. [16]) as follows:

$$S^{(4)}(\mathbf{r},t) = \frac{h_z^4}{4!}\times$$
$$\times \sum_{r_1\ldots r_4}\int d\tau_1\ldots d\tau_4 \langle T s_r^z(t) s_0^z(0) s_{r_1}^z(\tau_1)\ldots s_{r_4}^z(\tau_4)\rangle. \quad (7)$$

We are interested in the irreducible correlation function, so that we will have in mind that only irreducible diagrams should be taken into account.

It is convenient to introduce complex "bond fermions", defined on z-links as follows: $\psi_r = \frac{1}{2}(c_{r1} + i c_{r2})$ and $\phi_r = \frac{1}{2}(c^z_{r,1} + i c^z_{r,2})$, see Fig. 1. As

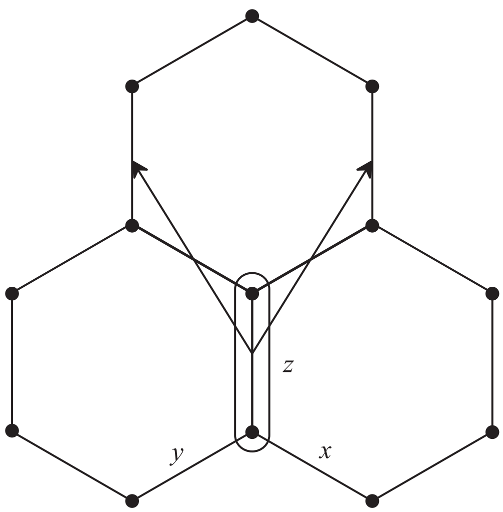

Fig. 1. A honeycomb lattice fragment: bond fermions ψ, ϕ belong to the z-link indicated on the figure

our representation of spin operator implies [14], each s^z inserts a Z_2 flux into neighbouring plaquetes. Hence, average in Eq. (7) does not vanish only if spin operators in this expression come in pairs, so that zero-flux state is obtained after all spin operators have been acting upon the ground state. These pairs of spin operators come in general at different time moments. However, for the time interval when such a flux exists in the intermediate state, a potential of the order of J for Majorana fermions is turned on [16]. Contribution of such an intermediate states is thus suppressed. This way, time indices become paired, too. In order to illustrate this mechanism, consider a contribution to the expression (7) for $r = r_1$, $r_2 = 0$, $r_3 = r_4 = \rho$. In terms of the bond fermions ($\psi_r^\alpha = (\psi, \psi^+)$, $\phi_r^\alpha = (\phi^+, \phi)$), this expression (for $t_1 < 0$) reads (analogously to [16]):

$$\langle T s_r^z(t) s_0^z(0) s_{r_1}^z(\tau_1)\ldots s_{r_4}^z(\tau_4)\rangle =$$
$$= 2^5 \langle e^{i\hat{H}t}\psi_r^{\alpha_1}\phi_r^{\alpha_1} e^{-i\hat{H}t}\psi_0^{\alpha_2}\phi_0^{\alpha_2} e^{i\hat{H}\tau_1}\psi_r^{\alpha_3}\phi_r^{\alpha_3} e^{-i\hat{H}\tau_1}\times$$
$$\times e^{i\hat{H}\tau_2}\psi_0^{\alpha_4}\phi_0^{\alpha_4} e^{-i\hat{H}\tau_2} e^{i\hat{H}\tau_3}\psi_\rho^{\alpha_5}\phi_\rho^{\alpha_5}\times$$
$$\times e^{-i\hat{H}\tau_3} e^{i\hat{H}\tau_4}\psi_\rho^{\alpha_6}\phi_\rho^{\alpha_6} e^{-i\hat{H}t}\rangle =$$
$$= -2^5 \langle e^{i\hat{H}t}\psi_r e^{-i\hat{H}_r t}\psi_0 e^{i\hat{H}_{r,0}\tau_1}\psi_r^+ e^{-i\hat{H}_0\tau_1}\times$$
$$\times e^{i\hat{H}_0\tau_2}\psi_0^+ e^{-i\hat{H}\tau_2} e^{i\hat{H}\tau_3}\psi_\rho e^{-i\hat{H}_\rho\tau_3} e^{i\hat{H}_\rho\tau_4}\psi_\rho e^{-i\hat{H}t}\rangle =$$
$$= 2^5 \langle T\psi_r(t)\psi_r^+(\tau_1)\psi_0(0)\psi_0^+(\tau_2)\psi_\rho(\tau_3)\times$$
$$\times \psi_\rho(\tau_4) e^{-i\int \hat{V}(\tau)d\tau}\rangle \quad (8)$$

with

$$V(\tau) = \theta(\tau-\tau_1)\theta(t-\tau)\hat{V}_r + \theta(\tau-\tau_2)\theta(0-\tau)\hat{V}_0 +$$
$$+ \theta(\tau-\tau_3)\theta(\tau_4-\tau)\hat{V}_\rho, \quad (9)$$

where $V_r = 4J\left(\psi_r^+\psi_r - \frac{1}{2}\right)$ and $H_r = H + V_r$. In the series of transformations shown in Eq. (8), we have used: i) the relation between spin and fermionic operators was used for the transformation from line *1* to line *2*, ii) commutation relations $\phi e^{iHt} = e^{iH_r t}\phi$ and $\phi^+ e^{iH_r t} = e^{iHt}\phi^+$ was used to transform line *2* into line *3*, and iii) identities $\phi^+\phi|0\rangle = \frac{1+u_{ij}}{2}|0\rangle$ and $e^{iHt}e^{-iH_r t} = Te^{-i\int V(\tau)d\tau}$ have been employed to obtain finally line *4*.

Following the standard route [21], we factorize the expression (8) as $2^5 e^C L$, where C stays for the sum of connected diagrams, $e^C = \langle Te^{-i\int \hat{V}(\tau)d\tau}\rangle$, and L stays for the contribution of "connected line". In the case of $t-\tau_1$ of the order of t this expression oscillates at high frequency $\sim J$, suppressing the value of the integral over τ_1. As a result, the dominating contribution is expected to come from a region of $t \approx \tau_1$, but if $t > 0 > \tau_1$, such a region is absent and the whole contribution in Eq. (8) is small. On the contrary, such a suppression does not occur for the region $t > \tau_1 > 0$. Here integration over τ_1 is equivalent to the substitution $\tau_1 \to t$ and multiplying the result by a additional factor $\frac{1}{h_0}$, where $h_0 \sim J$, see [16] for details.

All other pairings of spin operators can be considered similarly. As a result, the whole contribution to spin-spin correlation function of the order h_z^4 can be represented in the form of (the integral of) three-point correlation function of fermionic density:

$$\langle s_r^z(t) s_0^z(0)\rangle^{(4)} =$$
$$= 2^5\cdot 4\frac{h_z^4}{h_0^3}\sum_\rho \int d\tau \langle T\hat{n}^T(t,r)\hat{n}^T(0,0)\hat{n}^T(\tau,\rho)\rangle, \quad (10)$$

where $\hat{n}^T(t,r) = \hat{\psi}(t,r)\hat{\psi}^+(t,r)$. The factor of 4 result from two permutations of $s_t^z(r)$ and the paired spin operator giving the same contribution (the same for $s_0^z(0)$). Below we introduce short-hand notation $x = (\mathbf{r}, t)$.

Evaluation of the Fermionic correlation function. Writing $x = (r,t)$ it is convenient to define two Green functions [16]: $G(x) = \langle T\psi(x)\psi^+(0)\rangle = -\langle T\psi^+(0)\psi(x)\rangle$ and $F(x) = \langle T\psi(x)\psi(0)\rangle = \langle T\psi^+(0)\psi^+(x)\rangle$. Explicitely (for $t > 0$):

$$G(x) = \frac{-\sqrt{3}Jt(Z_1+Z_2) + (Z_2 - Z_1)r\cos\gamma}{4\pi(3J^2t^2 - r^2)^{3/2}} \quad (11)$$

and

$$F(x) = -i\frac{(Z_1+Z_2)r\sin\gamma}{4\pi(3J^2t^2 - r^2)^{3/2}}. \quad (12)$$

With these equations, the expectation value in expression (10) can be evaluated with the use of Wick theorem. Evaluation of the diagrams (see few examples in Fig. 2) requires calculation of convolutions of pairs of Green

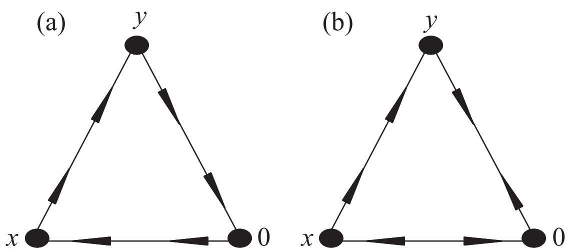

Fig. 2. Two types of diagrams, contributing to the fourth-order correction to the spin-spin correlation function

functions. As a result, combining all the contributions, we get for the density-density correlation function contribution of the order h_z^4:

$$S^{(4)}(\mathbf{r},t) = \frac{h_z^4}{2h_0^3}\frac{2^7}{(2\pi)^2\sqrt{3}}\frac{r\cos\gamma(Z_2^2 - Z_1^2)}{J(3J^2t^2 - r^2)^2} = = -i\frac{h_z^4}{h_0^3}\frac{2^7}{(2\pi)^2\sqrt{3}}\frac{r\cos\gamma\sin(\frac{2}{3}m\pi)}{J(3J^2t^2 - r^2)^2}. \quad (13)$$

Note that the ratio of the new contribution (13) to spin-spin correlation function to the lowest-order one given by Eq. (5), grows $\propto (h_z/J)^2 r$ at large distances. Therefore the result (13) is applicable at $r \ll (J/h_z)^2$.

Discussion. Perturbative contribution (13) can be reproduced by the addition of a vector potential $\mathbf{A}$ minimally coupled to the gradient term in the low-energy Fermionic Hamiltonian (4):

$$H_F = \sqrt{3}J\sum_{\mathbf{p}} \bar{a}_\lambda(\mathbf{p})\sigma^\alpha_{\lambda\mu}(p^\alpha - A^\alpha)a_\mu(\mathbf{p}), \quad \text{where} \quad \mathbf{A} = (-i\delta, 0), \quad (14)$$

with $\delta = \frac{2h_z^2}{\sqrt{3}h_0 J}$. The effective vector potential $\mathbf{A}$ was found to be purely imaginary. This apparently surprising result could be expected, since perturbation A_x is linearly coupled to the fermion density $\hat{n}^T(t,\mathbf{r})$ and should reproduce purely real result given by Eq. (10), by the first-order perturbation theory in $\mathbf{A}$.

We conjecture that replacement of low-energy effective Hamiltonian (4) by its extended version (14) with apppropriate vector potential $\mathbf{A}$ captures all effects of nonzero magnetic field as long as it has vanishing mixed product $h_x h_y h_z$. If generally correct, this result opens a way to study the effects of more complicated non-uniform (and also slowly time-varying) magnetic field configurations, including the effects of higher orders in h_z.

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