Spin-spin correlators in Majorana representation

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In the Majorana representation of a spin 1/2 we find an identity which relates spin-spin correlators to one-particle fermionic correlators. This should be contrasted with the straightforward approach in which two-particle (four-fermion) correlators need to be calculated. We discuss applications to the analysis of the dynamics of a spin coupled to a dissipative environment and of a quantum detector performing a continuous measurement of a qubit’s state.

I. INTRODUCTION

An analysis of spin dynamics involves calculations of spin correlators. Spin operators do not satisfy the Wick theorem, and various methods have been used to still enable the use of perturbative (diagrammatic) methods. One of the approaches is based on the Majorana-fermion representation of spin operators. This approach has a long history and was applied recently to condensed-matter problems.

In this approach one introduces three Majorana fermions $\eta_x, \eta_y, \eta_z$ (per spin) and expresses the (or Pauli) operators via these fermions:

\begin{align}
\sigma_x &= -i\eta_y\eta_z \\
\sigma_y &= -i\eta_z\eta_x \\
\sigma_z &= -i\eta_x\eta_y.
\end{align}

(1)

Obviously, an analysis of spin-spin correlations based on Eq. (1) requires calculations of a four-fermion correlator. In this note we show that spin correlators coincide with those of a four-fermion correlator. We discuss under which conditions this identity may simplify the analysis and discuss its particular applications.

II. MAJORANA REPRESENTATION

Majorana fermions satisfy the anti-commutation relations: $\eta_\alpha\eta_\beta = -\eta_\beta\eta_\alpha$ for $\alpha \neq \beta$ and $\eta_\alpha^2 = 1$, and are real: $\eta_\alpha = \eta_\alpha^\dagger$ ($\alpha, \beta, \gamma = x, y, z$). These properties ensure that the representation (1) reproduces the commutation relations of the spin algebra. An important feature of the representation (1) is the fact that the spin operators are bilinear (‘bosonic’) combinations of Dirac (annihilation / creation) fermionic operators.

One may construct the three Majorana fermion operators (for a spin) out of three different Dirac fermions, $\eta_\alpha = c_\alpha^\dagger + c_\alpha$, each annihilation operator acting in its own two-dimensional Hilbert space. This ensures the anti-commutation relations and the property $\eta_\alpha^2 = 1$. The whole Hilbert space is then 8-dimensional.

The dimensionality of the Hilbert space may be reduced if two Majorana fermions, e.g. $\eta_x$ and $\eta_y$, are constructed as linear combinations of a single Dirac fermion $f$ and its conjugate $f^\dagger$: $\eta_x = f + f^\dagger$ and $\eta_y = i(f^\dagger - f)$.

Another Dirac fermion $g = c_z$ is still needed to construct the third Majorana fermion $\eta_z = g + g^\dagger$. In this mixed Majorana-Dirac picture

\begin{align}
\sigma_+ &= \eta_zf \\
\sigma_- &= f^\dagger\eta_z \\
\sigma_z &= 1 - 2f^\dagger f.
\end{align}

(2)

This ‘drone-fermion’ representation was used for the analysis of magnetic systems in the 60s (see Refs. [1,2,3]). The whole Hilbert space in this representation is 4-dimensional. Depending on the rotational symmetry, this representation may be more convenient than (1).

We have described this construction in the Hilbert space of two Dirac fermions $f$ and $g$. Alternatively one can view it as two replicas of the original spin. Indeed, let us label the basis states in the following way: denote the state without $f$- and $g$-fermions by $|00\rangle \equiv |0\rangle$, and also $|01\rangle \equiv |g\rangle |0\rangle$, $|10\rangle \equiv f^\dagger |0\rangle$, and $|11\rangle \equiv f^\dagger g^\dagger |0\rangle$. For the state $|n\rangle$ the first index $s = \uparrow / \downarrow$ denotes the spin component, while the second $n = a/b$ labels the spin copy. One notices that the spin operators $\sigma_+, \sigma_-,$ and $\sigma_z$ do not mix the $a$- and $b$-subspaces, i.e., they operate in the same way on the two ‘copies’ of the spin. Further, one may view the index $n = a/b$ as an isospin and introduce the respective Pauli isospin operators $\tau_x, \tau_y, \tau_z$. In particular, $\tau_x$ is the ‘copy-switching’ operator: $\tau_x |s_a\rangle = |s_b\rangle$ and $\tau_x |s_b\rangle = |s_a\rangle$. The fermionic operators can be expressed as

\begin{align}
f = \sigma_+\tau_x, \quad f^\dagger = \sigma_-\tau_x, \quad \eta_z = \sigma_z\tau_x.
\end{align}

(3)

Further, $\eta_\alpha = \sigma_\alpha\tau_x$, for any $\alpha = x, y, z$. Accordingly, in terms of the fermionic operators we have $\tau_x = (1 - 2f^\dagger f)\eta_z = -i\eta_x\eta_y\eta_z$. The operator $\tau_x$ commutes with all ‘other’ operators: with $\sigma_+, \sigma_-, \sigma_z, f, f^\dagger, \eta_z$.

III. REDUCTION OF THE SPIN-SPIN CORRELATORS

A physical Hamiltonian depends on the spin operators $\sigma_x, \sigma_y, \sigma_z$ (and on other degrees of freedom, e.g., the electrons in the Kondo problem). Thus the operator $\tau_x$ commutes with any Hamiltonian and we obtain

\begin{align}
\langle \sigma_\alpha(t)\sigma_\beta(t') \rangle = \langle \tau_x(t)\eta_\alpha(t)\tau_x(t')\eta_\beta(t') \rangle = \langle \eta_\alpha(t)\eta_\beta(t') \rangle.
\end{align}

(4)
Here we have used the fact that $\tau_x$ is time-independent, commutes with the Majorana fermions, and that $\tau_x^2 = 1$. For example, we obtain

$$
\langle \sigma_x(t)\sigma_x(t') \rangle = \langle \eta_x(t)\eta_x(t') \rangle = \langle [f(t) + f^\dagger(t)][f(t') + f^\dagger(t')] \rangle .
$$

(5)

In certain situations the identity (5) may simplify the calculations. Indeed, if the Majorana representation (1), (2) is used for a calculation of spin-spin correlations, a four-fermion correlator needs to be evaluated. In a typical situation, the lowest-order contribution is given by a loop-like diagram which involves two fermionic propagators. A straightforward evaluation of higher-order contributions requires an analysis of the self-energy corrections to these propagators as well as of the vertex corrections. The use of the relation (4) reduces the task to the evaluation of a single self-energy.

In general, evaluation of this self-energy to all orders in the perturbative expansion involves complicated diagrams and, in particular, other self-energies and vertex corrections. Hence an involved calculation may still be needed. Nevertheless, the relation (4) may be useful if the needed self-energy part can be estimated reliably, for instance, by calculating the low-order contributions. We discuss two examples in Section V.

Note also that the relation (4) may be straightforwardly generalized to multi-spin correlators, the evaluation of which then reduces to multi-fermion correlators. Further, in a problem, that involves many spins represented via Majorana fermions, (e.g., a lattice spin model) the $\tau_x$-operators for different spins (sites) may be involved in a relation similar to (4). In this case their product does not drop out of the calculation (unlike $\tau_x^2 = 1$ for one spin).

IV. GAUGE-INVARINANCE CONSIDERATIONS

One might be concerned by the fact that Eq. (4) reduces a correlator of physical quantities to a correlator of “unphysical” operators. Another way of expressing this concern is to invoke the gauge symmetry. Indeed the Majorana representations (1) and (2) possess the discrete $Z_2$-symmetry $\eta_x \to -\eta_x$. As an operator which realizes the symmetry transformation one may choose $\tau_y = i(g^\dagger - g)$ (cf. Ref.11). For example, $\eta_z \to \tau_y \eta_z \tau_y^{-1} = -\eta_z$. Thus, the forth Majorana fermion allowed in the Hilbert space of the representation (2) generates the symmetry transformation. One can as well use as a generator $\tau_z$, which just flips the sign of the wave function of the b-spin, keeping that of the a-spin intact.

Consider now a time-dependent gauge transformation, which transforms a wave function $|\Psi\rangle$ to $U|\Psi\rangle$, where

$$
U = \exp \left( \frac{i\pi}{2} \tau_y \phi(t) \right)
$$

(6)

and $\phi(t) = 0, 1$. It transforms the operators $\eta_x \to (-1)^{\phi(t)}\eta_x$, $\tau_x \to (-1)^{\phi(t)}\tau_x$. Thus the operator $\tau_x$ is now time-dependent and no longer commutes with the Hamiltonian. Indeed, the gauge-transformed Hamiltonian reads

$$
\hat{H} = UHU^{-1} + i\dot{U}U^{-1} = H - \frac{\pi}{2} \phi(t)\tau_y ,
$$

(7)

and the last (gauge) term does not commute with $\tau_x$. Thus we find that

$$
\langle \eta_\alpha(t)\eta_\alpha(t') \rangle \to (-1)^{\phi(t)-\phi(t')}\langle \eta_\alpha(t)\eta_\alpha(t') \rangle ,
$$

(8)

i.e., the single-fermion correlators are not gauge-invariant.

V. APPLICATIONS

The relation (4) can simplify calculations, since to evaluate a single-fermion Green function one needs only to evaluate a self-energy. In a perturbative regime, when one may restrict oneself to evaluating the lowest-order contribution, Eq. (4) simplifies the task.

One example of such a problem is dicussed in Ref.9 where continuous measurement of the state of a spin (qubit) by a quantum detector is analyzed and the output noise of the detector as well as the spin dynamics is studied. A calculation of a spin-spin correlator in the Majorana representation requires an evaluation of a two-fermion loop and involves the analysis of two self-energy parts and a vertex correction. It turns out that the vertex correction is important already in the lowest order and may even cancel one of the self-energy contributions. This fact may be understood and the calculations are considerably simplified if the relation (4) is invoked. The obtained result coincides with an alternative calculation, in which instead of using the Majorana representation to enable the use of the Wick theorem one follows the dynamics of the spin directly. This approach may be useful if the problem involves only a small number of spins (or other ‘non-Wick’ degrees of freedom).

Here we consider another example: the dissipative dynamics of a spin coupled to an environment, for instance, the spin-boson model. Consider the case of a purely transverse coupling:

$$
H = -\frac{1}{2} B \sigma_z - \frac{1}{2} X(t) \sigma_x + H_{bath} ,
$$

(9)
where $X$ is a fluctuating bosonic observable of the bath, whose Hamiltonian $H_{\text{bath}}$ determines the statistics of fluctuations. We consider gaussian, but not necessarily equilibrium, fluctuations. Using the Keldysh technique we perform a calculation considering the bath-spin coupling (the second term on the rhs of Eq. (9)) as a perturbation.

Below we use the notations of Ref. [1]. Let us introduce the matrix Green function of the bath:

$$G_X = -i\langle T_K X(t)X(t') \rangle$$

(10)

Its Keldysh component

$$G^K_X = G^>_X + G^<_X = -2iS_X \ ,$$

(11)

and the difference between the retarded and advanced components

$$G^R_X - G^A_X = G^>_X - G^<_X = -2iA_X \ ,$$

(12)

are related to the symmetrized and antisymmetrized correlators: $(X(t)X(0)) \equiv S_X(t) + A_X(t)$, $S_X(-t) = S_X(t)$, $A_X(-t) = -A_X(t)$. In equilibrium they are related by the fluctuation-dissipation theorem: $S_X(\omega) = A_X(\omega) \coth(\hbar\omega/2k_BT)$. Here $G^>_X = -i\langle X(t)X(0) \rangle$ and $G^<_X = -i\langle X(0)X(t) \rangle$.

Similarly, for the Majorana fermion $\eta \equiv \eta$, we define $G_\eta \equiv -i\langle T_K \eta \eta(t') \rangle$. The bare Green functions are $G^R_{\eta,0} = -i$ and $G^A_{\eta,0} = i$. For the $f$-fermion we use the Bogolubov-Nambu spinors $\Psi \equiv (f, f^\dagger)^T$ and $\Psi^\dagger \equiv (f^\dagger, f)$ and define a matrix $G_\Psi \equiv -i\langle T_K \Psi(t)\Psi^\dagger(t') \rangle$.

Calculation of the spin propagators (in a stationary state) reduces due to the relation to the evaluation of the fermion Green functions $G_\Psi$ and $G_\eta$. These functions can be found from the Dyson (kinetic) equations:

$$G_\Psi^{-1} = G^R_{\Psi,0} - \Sigma_\Psi \ ,$$

(13)

$$G_\eta^{-1} = G^R_{\eta,0} - \Sigma_\eta \ ,$$

(14)

where $\Sigma_\Psi$ and $\Sigma_\eta$ are the self-energies. All the quantities in Eqs. (13) are $4 \times 4$ matrices (with the Nambu and Keldysh components). In the frequency domain the operator $G_{\Psi,0}$ is given by

$$G_{\Psi,0}^{-1} = \begin{pmatrix} \omega - B & 0 & 0 & 0 \\ 0 & \omega + B & 0 & 0 \\ 0 & 0 & \omega - B & 0 \\ 0 & 0 & 0 & \omega + B \end{pmatrix}$$

(15)

while for $G_{\eta,0}$ we obtain

$$G_{\eta,0}^{-1} = \begin{pmatrix} \omega/2 & 0 & 0 \\ 0 & \omega/2 \end{pmatrix}$$

(16)

We disregard infinitesimal imaginary terms in Eqs. (13) since they are superseded by the self-energy parts in Eqs. (13) [14].

The lowest-order contributions to the self-energies are shown in Fig. 1 (the matrix structure after the first diagram in Fig. 1, we find

$$\Sigma_\Psi = \begin{pmatrix} \Sigma_\Psi^R & \Sigma_\Psi^A \end{pmatrix}, \quad \Sigma_\eta = \begin{pmatrix} \Sigma_\eta^R & \Sigma_\eta^A \end{pmatrix}$$

(17)

are shown in Fig. 1 (the matrix structure after the Keldysh rotation is given in 11,12). We find that

$$\Sigma_\Psi^R = (i/4)\lambda G^R_X G^R_\eta \quad \text{and} \quad \Sigma_\Psi^A = (i/4)\lambda G^A_X G^A_\eta$$

where $\lambda = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$ is a matrix in the Nambu space. Similarly, we obtain

$$\Sigma_\eta^R = (i/4)G^R_X \begin{pmatrix} 1 & -1 \end{pmatrix} G^R_\eta \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

and

$$\Sigma_\eta^A = (i/4)G^A_X \begin{pmatrix} 1 & -1 \end{pmatrix} G^A_\eta \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$  

While the retarded and advanced components of the bare fermion Green functions are known, its Keldysh component contains information about the distribution function and is sensitive to the environment (cf. Ref. [14]).

To perform the calculation, one introduces the distribution function $h_\eta$ via $G^R_\eta(\omega) = h_\eta(\omega) (G^R_X(\omega) - G^A_X(\omega))$. Evaluating $\Sigma_\Psi$ from the first diagram in Fig. 1 we find

$$\Sigma_\Psi^R(\omega) - \Sigma_\Psi^A(\omega) = \frac{\lambda}{4} \left[ G^R_X(\omega) + h_\eta(0)(G^R_X(\omega) - G^A_X(\omega)) \right] \ ,$$

(18)

$$\Sigma_\Psi^K(\omega) = \frac{1}{4} \lambda \left[ (G^R_X(\omega) - G^A_X(\omega)) + h_\eta(0)G^K_X(\omega) \right] \ ,$$

(19)

The symmetry relation $h_\eta(-\omega) = -h_\eta(\omega)$ implies $h_\eta(0) = 0$. Hence without evaluating $h_\eta$ we find

$$\Sigma_\Psi^R(\omega) - \Sigma_\Psi^A(\omega) = -i \frac{\lambda}{2} S_X(\omega) \ ,$$

(20)

and

$$\Sigma_\Psi^K(\omega) = -i \frac{\lambda}{2} A_X(\omega) .$$

(21)

The real parts of the retarded and advanced self-energies give the non-equilibrium generalization of the Lamb shift,
i.e., renormalize the level splitting $B$. This renormalization is small if the noise is weak and has a non-singular spectrum.

Substituting the self-energy $\Sigma_\psi$ into the Dyson equation \[ G^{-1}_\psi = G^{-1}_{\psi,0} - \left( \begin{array}{ccc} -i\Gamma(\omega) & i\Gamma(\omega) & -iA_X(\omega)/2 & iA_X(\omega)/2 \\ i\Gamma(\omega) & -i\Gamma(\omega) & iA_X(\omega)/2 & -iA_X(\omega)/2 \\ 0 & 0 & i\Gamma(\omega) & -i\Gamma(\omega) \\ 0 & 0 & i\Gamma(\omega) & i\Gamma(\omega) \end{array} \right), \] (22)

where $\Gamma(\omega) \equiv S_X(\omega)/4$. Inverting Eq. (22) we obtain

\[ G^{R/A}_\psi = \left( \begin{array}{ccc} \omega + B \pm i\Gamma(\omega)/2 & \pm i\Gamma(\omega) & 0 \\ \pm i\Gamma(\omega) & \omega - B \pm i\Gamma(\omega)/2 & 0 \\ 0 & 0 & 1 \end{array} \right), \] (23)

\[ G^K = \frac{i}{2} \left( \begin{array}{cc} 0 & \omega^2 - B^2 \\ \omega^2 - B^2 & 0 \end{array} \right), \] (24)

From Eqs. (23) and (24) we see that, at least in this order of perturbation theory, we can use the relation $G^K = h_\psi(\omega) (G^K_{\psi,0} - G^K_{\psi,0})$, where $h_\psi(\omega) = -h_\psi(\omega)$ and (for any pair $ij$ of Nambu indices)

\[ h_\psi(\omega) = \frac{\Sigma^K_{\psi,ij}(\omega)}{\Sigma^K_{\psi,ij}(\omega)} = \frac{A_X(\omega)}{S_X(\omega)}, \] (25)

a quantity of the zeroth order in the coupling constant.

Using these results we can calculate $\Sigma^K_{\eta,0} = 0$:

\[ \Sigma^K(\omega) = \frac{1}{S} \left( \Sigma^K_{\psi,0}(\omega) - \Sigma^K_{\psi,0}(\omega) \right) + h_\psi(\omega)(G^K_{\psi,0}(\omega - B) - G^K_{\psi,0}(\omega - B)) \]

\[ + [B \rightarrow -B], \] (26)

\[ \Sigma^K = \frac{1}{S} \left( (G^K_{\psi,0}(\omega - B) - G^K_{\psi,0}(\omega - B)) \right) + h_\psi(\omega)(G^K_{\psi,0}(\omega - B)) + [B \rightarrow -B]. \] (27)

We evaluate the self-energy $\Sigma_\eta$ near the pole $\omega = 0$ of the Green function $G_\eta$:

\[ \Sigma^K_\eta(0) = 0 \] (28)

and

\[ \Sigma^K(0) - \Sigma^K(0) = -iS_X(B) \left( 1 - \frac{A_X^2(B)}{S_X^2(B)} \right). \] (29)

Now, with the acquired knowledge of single-fermion Green functions, we can evaluate various spin-spin correlators. We start with

\[ \Pi_{xx} = -i(T_K\sigma_x(t)\sigma_x(t')) = \left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right). \] (30)

where the bosonic time-ordering is chosen for the spin components. From Eq. (11) we deduce that

\[ \Pi^K_{xx} = -i\langle \sigma_x(t)\sigma_x(t') \rangle = \left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right). \] (31)

Since $G^K = \frac{1}{2}[G^K_{\psi} + G^K_{\psi} - G^K_{\psi}]$, we obtain

\[ i\Pi^K_{xx} = \left( \begin{array}{cc} \frac{1}{2}S_X(B) + A_X(\omega)/2 \\ -\frac{1}{2}S_X(B) - A_X(\omega)/2 \end{array} \right), \] (32)

This result describes the peaks in the spectrum of spin correlations at $\omega = \pm B$, with the width corresponding to the dephasing rate $T_2^{-1} = \Gamma(B) = S_X(B)/4$, thus reproducing the form known, e.g., from the analysis of the Bloch-Redfield equations. \[ \Pi^K_{xx} = \left( \begin{array}{cc} \frac{1}{2}S_X(B) + A_X(\omega)/2 \\ -\frac{1}{2}S_X(B) - A_X(\omega)/2 \end{array} \right). \] (33)

Similarly, for the Green function of the Majorana fermion $\eta$ we obtain

\[ G^K_{\eta} = \frac{1}{\omega + 2i\Gamma}, \] (34)

where

\[ \Gamma = \frac{S_X(B)}{4} \left( 1 - \frac{A_X^2(B)}{S_X^2(B)} \right). \] (35)

The Keldysh component vanishes, $G^K_\eta = 0$, and we find

\[ i\Pi^K_{xx} = \langle \sigma_z(t)\sigma_z(t') \rangle = iG^K_{\eta} = \frac{i\Gamma}{\omega^2 + 4\Gamma^2}. \] (36)

This may be compared to the peak shape obtained in the Bloch-Redfield approach. It can be expressed in terms of the average value $\langle \sigma_z \rangle = A_X(B)/S_X(B)$ of the $z$-component:

\[ i\Pi^K_{xx} = \langle \sigma_z \rangle^2 2\pi\delta(\omega) + \left( 1 - \langle \sigma_z \rangle^2 \right) \frac{2T_2^{-1}}{\omega^2 + T_1^{-2}}, \] (37)

where the relaxation time is given by $T_1^{-1} = 2T_2^{-1}$. The result (37) reproduces the high-frequency behavior of Eq. (36) and the ‘width of the peak’, which may be read off from the high-$\omega$ asymptotics, $i\Pi_{xx} \sim 2(1 - \langle \sigma_z \rangle^2)/(T_1\omega^2)$. This indicates that at lower frequencies higher-order corrections (contributions to $\Sigma^K_\eta$) are important, which requires a further analysis.

VI. SUMMARY

In summary, we discussed an identity relating spin correlations to single-particle Majorana-fermion propagators and problems where the use of this relation simplifies the analysis.

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