Emergence of multiple Higgs modes due to spontaneous breakdown of a $\mathbb{Z}_2$ symmetry in a superconductor

Shunji Tsuchiya

1Department of Physics, Chuo University, 1-13-27 Kasuga, Bunkyo-ku, Tokyo 112-8551, Japan

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We study the Higgs mode in a Bardeen-Cooper-Schrieffer (BCS) superconductor. Motivated by the observation that $U(1)$ symmetry of the BCS Hamiltonian is not essential for the Higgs mode, we study the Ising-like Hamiltonian in the pseudospin representation. We show that the Higgs mode emerges as the lowest excited state of the Ising-like Hamiltonian due to spontaneous breakdown of $Z_2$ symmetry under the time-reversal operation $\mathcal{T}$ in the pseudospin space. We further predict the existence of multiple Higgs modes that have quantized energy $2(n+1)\Delta_0$ ($0 \leq n \leq N_{k_F}$), where $\Delta_0$ is the superconducting gap, $n$ is an integer, and $N_{k_F}$ is the number of states on the Fermi surface.

Introduction.—Higgs modes and Nambu-Goldstone (NG) modes are ubiquitous collective excitations that arise in systems with spontaneous symmetry breaking $\mathbb{Z}_2$. They are amplitude and phase modes of the order parameter and appear in a broad class of systems in condensed-matter and particle physics. Stimulated by the discovery of the Higgs boson in the Standard Model $\mathbb{Z}_2$, interests in Higgs modes in condensed-matter physics have grown recently [7, 8]. Higgs modes have been observed in various condensed-matter systems including superconductors [9–15], superfluids [16–18], quantum spin systems [19–22], charge-density-wave (CDW) materials [23, 24], and ultracold atomic gases [25, 26].

Although Higgs modes are believed to emerge with NG modes when continuous symmetries are spontaneously broken, fundamental questions on Higgs modes remain to be understood. Namely, in contrast with NG modes, whose existence is predicted by the Goldstone theorem $\mathbb{Z}_2$, Higgs modes do not necessarily appear in systems exhibiting spontaneous breakdown of continuous symmetries. For instance, whereas a Higgs mode appears in a Bardeen-Cooper-Schrieffer (BCS) superconductor $\mathbb{Z}_2$, it disappears in a Bose-Einstein condensate (BEC) $\mathbb{Z}_2$, although spontaneous breakdown of $U(1)$ symmetry occurs in both systems and, furthermore, the former continuously evolves to the latter in the BCS-BEC crossover phenomenon $\mathbb{Z}_2$.

Particle-hole (p-h) symmetry is a crucial condition for the emergence of Higgs modes. In superconductors, for instance, Higgs modes appear when the fermion energy dispersion is p-h symmetric $\mathbb{Z}_2$. In a bosonic superfluid in an optical lattice, the system exhibits the approximate p-h symmetry in the vicinity of the tip of the Mott lobe, where a Higgs mode appears $\mathbb{Z}_2$.

In the previous work $\mathbb{Z}_2$, we have shown that the BCS Hamiltonian for a superconductor with a p-h symmetric fermion energy dispersion has the non-trivial $Z_2$ symmetries under discrete operations. We refer to them as the charge-conjugation ($C$), parity ($P$), and time-reversal ($T$) operations in analogy with the corresponding ones in the relativistic field theory $\mathbb{Z}_2$. We found that $T$ and $P$ are spontaneously broken, while $C$ is unbroken in the BCS ground state. We further conjectured that the emergence of the Higgs mode may be a consequence of the spontaneous breakdown of $Z_2$ symmetry under $T$.

In this Letter, extending the previous work, we establish that the Higgs mode emerges in a superconductor due to spontaneous breakdown of $Z_2$ symmetry under $T$. Motivated by the observation that $U(1)$ symmetry is not essential for the Higgs mode, we study the Ising-like Hamiltonian in the pseudospin representation $H_I$ derived from the BCS Hamiltonian, which exhibits $Z_2$ symmetries under $C$, $P$, and $T$. We show that the Higgs mode appears as the lowest excited state of $H_I$ due to spontaneous breakdown of $Z_2$ symmetry under $T$ in the ground state. Furthermore, we predict the existence of the multiple Higgs modes that have quantized energy $2(n+1)\Delta_0$ ($0 \leq n \leq N_{k_F}$) and include the original one ($n = 0$), where $\Delta_0$ is the superconducting (SC) gap, $n$ is an integer, and $N_{k_F}$ is the number of states on the Fermi surface (FS). Our main results are schematically illustrated in Fig. 1 (a).

Particle-hole symmetry and Higgs modes.—To illustrate
the condition in which the Higgs mode is well-defined in a superconductor, let us first discuss the relation between p-h symmetry and the Higgs mode. For simplicity, we consider the BCS Hamiltonian in the pseudospin representation \[1, 42\]

\[
\mathcal{H}_{BCS} = \mathcal{H}_K + \mathcal{H}_{XY}, \quad \mathcal{H}_K = \sum_k 2\xi_k S_{z,k},
\]

\[
\mathcal{H}_{XY} = -g \sum_{k,k'} (S_{z,k} S_{z,k'} + S_{y,k} S_{y,k'})
\]

where \( S_k = (S_{z,k}, S_{y,k}, S_{z,k}) \) is the spin-1/2 pseudospin operator and \( S_\mu = \sum_k S_{\mu,k} \) is the total spin. We set \( h = 1 \) throughout the Letter. The fermion vacuum corresponds to the spin-down state \((0)_k = |↓\rangle_k\) and the fully occupied state to the spin-up state \((c_k^+ c_{-k}^- |0\rangle_k = |↑\rangle_k\)

where \( c_k^+ \) is the creation operator for a fermion with momentum \( k \) and spin \( s(=\uparrow, \downarrow) \). \( \mathcal{H}_K \) is the kinetic energy term and \( \mathcal{H}_{XY} \) is the interaction term. Here, \( \xi_k = \varepsilon_k - \mu \) is the energy dispersion of a fermion measured from the chemical potential \( \mu \) and \( g(>0) \) is the coupling constant for the attractive interaction between fermions. We do not specify the form of \( \varepsilon_k \) for generality of argument.

\( \mathcal{H}_{BCS} \) has rotational U(1) symmetry about the z-axis in the pseudospin space that reflects U(1) gauge symmetry. It is spontaneously broken in the SC state \[1, 2\]. When \( \xi_k \) satisfies the condition for the p-h symmetry

\[
-\xi_k = \xi_k, \quad (3)
\]

\( \mathcal{H}_{BCS} \) has additional \( \mathbb{Z}_2 \) symmetries under \( C \) and \( T \) \[42\]. Here, \( k \) and \( \bar{k} \) are a pair of wave vectors that are located on the opposite side of the FS with the same distance from it (See Figs. 1 (a)-(c) in Ref. \[42\]). \( C, P \), and \( T \) are defined as

\[
C = \mathcal{F} \prod_k \sigma_{z,k}, \quad \mathcal{F} = \prod_k f_{k, \bar{k}}, \quad (4)
\]

\[
T = U_T K, \quad U_T = \mathcal{F} \prod_k (-i \sigma_{y,k}), \quad (5)
\]

\[
P = \prod_k \sigma_{z,k}, \quad (6)
\]

where \( \prod_k = \prod_{\xi_k > 0} \sigma_{z,k} \equiv 2S_{\mu,k} \), \( f_{k, \bar{k}} \) is a swapping operator between the states of \( k \) and \( \bar{k} \), and \( K \) is the complex conjugation operator. Note that \( P \) represents a \( \pi \) rotation about the z-axis that is an element of U(1). \( \mathcal{CPT} \) and all other permutations of \( C, P, \) and \( T \) are exact symmetries. \( \mathbb{Z}_2 \) symmetries under \( T \) and \( P \) are spontaneously broken with U(1) in the SC state, while that under \( C \) is unbroken \[42\].

On the other hand, the Higgs mode appears as an amplitude mode only when \( \xi_k \) is p-h symmetric, i.e., it satisfies Eq. \[3 x 42\]. In the classical spin analysis, for a gap function in the ground state \( \Delta_0 > 0 \), amplitude and phase fluctuations of the gap function are proportional to those of the \( x \) and \( y \) components of the total spin as \( \delta \Delta \propto \delta S_x \) and \( \delta \theta \propto \delta S_y \), respectively. \( \delta \Delta \) and \( \delta \theta \) are uncoupled and pure amplitude oscillations of the Higgs mode are allowed only when \( \xi_k \) is p-h symmetric, because the off-diagonal element of the dynamical spin susceptibility \( \chi_{xy}(\omega) \) vanishes due to the opposite parity of \( S_x \) and \( S_y \) under \( C \) \[42, 44\]. When \( \xi_k \) is not p-h symmetric, finite \( \chi_{xy}(\omega) \) couples amplitude and phase fluctuations.

Moreover, the Higgs mode is stable only when \( \xi_k \) is p-h symmetric \[42\]. It is prohibited to decay into single-particle excitations despite its degeneracy with the lower edge of the single-particle continuum at \( 2\Delta_0 \), because the Higgs mode has even parity and the single-particle excitations at \( 2\Delta_0 \) have odd parity under \( C \). When \( \xi_k \) is not p-h symmetric, however, the Higgs mode merges with the single-particle continuum and suffers from strong damping due to decay into single-particle excitations. Thus, the Higgs mode is well-defined only when \( \mathbb{Z}_2 \) under \( T \) is spontaneously broken with U(1) in the SC state.

\textbf{Minimal Hamiltonian for Higgs modes}.— To argue the origin of the Higgs mode, we focus on a p-h symmetric system, in which the Higgs mode is well-defined, and assume Eq. \[6 \] in the rest of the Letter.

In the classical spin analysis, one finds that the \( y \) component of the interaction term \( \mathcal{H}_Y = -g S_y^2 \) may be irrelevant to the Higgs mode, because the Higgs mode involves out-of-phase oscillations of \( \delta S_y \) and \( \delta S_y \), whereas \( \mathcal{H}_Y \) induces in-phase oscillations of them \[42, 44\]. Furthermore, the analysis based on the Holstein-Primakoff (H-P) theory suggests that \( \mathcal{H}_Y \) is not necessary for constructing the creation operator of the Higgs mode \[42\]. Motivated by these observations, we neglect \( \mathcal{H}_Y \) and study the Ising-like Hamiltonian \( \mathcal{H}_I \):

\[
\mathcal{H}_I = \mathcal{H}_K + \mathcal{H}_X, \quad (7)
\]

\[
\mathcal{H}_X = -g \sum_{k,k'} S_{z,k} S_{z,k'} = -g S_z^2, \quad (8)
\]

Note that \( \mathcal{H}_I \) is invariant under \( C, P \), and \( T \), despite it loses U(1) symmetry. We derive the Higgs mode from \( \mathcal{H}_I \) to demonstrate that the emergence of the Higgs mode is not due to spontaneous breakdown of U(1) but to that of \( \mathbb{Z}_2 \) under \( T \).

\textbf{Discrete symmetries of \( \mathcal{H}_I \).—} In addition to \( \mathbb{Z}_2 \) symmetries under \( C, P \), and \( T \), \( \mathcal{H}_I \) has \( \mathbb{Z}_2 \) symmetries under local charge-conjugation operations in momentum space \( \mathcal{C}_{k,k'} = f_{k,k'} \sigma_{z,k} \sigma_{z,k'} \) and \( \mathcal{C}_{k,k} = \sigma_{z,k} \), where \( C \) can be written as \( C = \prod_k \mathcal{C}_{k,k} \otimes \prod_{k,y} \mathcal{C}_{y,y} \). To prove the invariance under \( \mathcal{C}_{k,k} \), it is convenient to introduce a pseudospin operator

\[
S_{\mu,k} = S_{\mu,k} - (-1)^{\delta \mu \cdot z} S_{\mu,k'}, \quad (9)
\]

where \( k \) is above the FS (\( \xi_k > 0 \)). It commutes with \( \mathcal{C}_{k,k} \).

The kinetic energy term can be written as

\[
\mathcal{H}_K = \sum_k 2\xi_k S_{z,k}, \quad (10)
\]
where \( \sum_{k} \equiv \sum_{\xi_k > 0} \). We obtain \([\mathcal{H}_K, C_{kk'}] = [\mathcal{H}_K, C_{kF}] = 0\) from Eq. (10). Since \( S_x = \sum_k S_x^k = \sum_{k_F} S_x^k \), \( S_x^k \) commutes with either \( C_{kk'} \) and \( C_{kF} \), we also obtain \([\mathcal{H}_X, C_{kk'}] = [\mathcal{H}_X, C_{kF}] = 0\) and \([\mathcal{H}_I, C_{kk'}] = [\mathcal{H}_I, C_{kF}] = 0\). Consequently, \( \mathcal{H}_I \) has \( Z_2 \) symmetry under each of \( C_{kk'} \) and \( C_{kF} \). \( \mathcal{H}_Y \) and \( \mathcal{H}_{BCS} \), in contrast, commute with neither \( C_{kk'} \) nor \( C_{kF} \).

**Discrete symmetries in low-energy states of \( \mathcal{H}_I \).**—We next study the symmetry of the ground state of \( \mathcal{H}_I \). The pseudospin configuration of it is shown in Fig. 1(b). The pseudospins turn smoothly from up to down towards either positive or negative \( x \)-direction as \( k \) evolves from below to above the FS, where the gap function \( \Delta \equiv g(S_x) \) is positive and negative in the former and latter cases, respectively. One of them being chosen spontaneously, \( Z_2 \) under \( \mathcal{P} \) is broken in the ground state. It leads to breakdown of \( Z_2 \) under \( \mathcal{T} \) due to unbroken \( Z_2 \) under \( \mathcal{C} \), which is shown below, and the exact symmetry under \( CPT \).

The energy landscape of \( \mathcal{H}_I \) is effectively described by the double-well potential, as schematically illustrated in Fig. 1(a).

Let us show that \( Z_2 \) under each of \( C_{kk'}, C_{kF} \), and \( \mathcal{C} \) is unbroken in the ground state. If we introduce a gap function \( \Delta = \Delta_0 > 0 \), \( \mathcal{H}_I \) reduces to the mean-field (MF) Hamiltonian

\[
\mathcal{H}_{MF} = \sum_k 2E_k S'_{sk} = \sum_k 2E_k S'_k + 2\Delta_0 \sum_{k_F} S_{zkF} \tag{11}
\]

where \( E_k = \sqrt{\xi_k^2 + \Delta_0^2} \) is the dispersion of a single-particle excitation referred to as a bogolon. \( S'_{sk} \) is the pseudospin operator for a pair of bogolons with \( |\uparrow\rangle_k \) and \( |\downarrow\rangle_k \) being the eigenstates of \( S'_k \) \([13,42,44]\). Note that \( \mathcal{H}_I \) and \( \mathcal{H}_{BCS} \) reduce to the same MF Hamiltonian for a real gap function. Here, we have introduced a spin operator

\[
S'_{\mu kk} = S'_{\mu k} - (-1)^{\beta_{\mu \nu}} S'_{\mu k}, \quad (\mu = x, y, z), \tag{12}
\]

where \( k \) is above the FS (\( \xi_k > 0 \)). It commutes with \( C_{kk'} \).

Using Eq. (11), we obtain \([\mathcal{H}_{MF}, C_{kk'}] = [\mathcal{H}_{MF}, C_{kF}] = 0\). Consequently, \( Z_2 \) symmetry under each of \( C_{kk'} \) and \( C_{kF} \) as well as under \( \mathcal{C} \) is unbroken in the ground state of \( \mathcal{H}_I \).

The eigenstates of \( \mathcal{H}_{MF} \) can be characterized by parity under \( C_{kk'} \) and \( C_{kF} \). The ground state of Eq. (11) \( |\Psi\rangle = \prod_k |\uparrow\rangle \bigotimes \prod_{k_F} |\uparrow\rangle \bigotimes 1 \rangle \) has even parity for all \( C_{kk'} \) and \( C_{kF} \), where \( \bigotimes \equiv (|\uparrow\rangle \bigotimes |\downarrow\rangle \bigotimes \sqrt{2} \). Here, the product states \( |s', t'\rangle_{kk'} = |s'\rangle_k \bigotimes |t'\rangle_{k_F} \) (\( s, t = \uparrow, \downarrow \)) are decomposed into the even and odd parity states under \( C_{kk'} \), where the former consist of the spin-1 triplet states \( |m\rangle_{kk'} \) \((m = 1, 0, -1)\) for \( S'_{\mu kk} \) and the latter the spin-0 singlet state \( |0\rangle_{kk'} \tag{44} \). The group state \( |\Psi\rangle = \mathcal{T} |\Psi\rangle \) for \( \Delta = -\Delta_0 \) has even and odd parity under \( C_{kk'} \) and \( C_{kF} \), respectively.

Parity of single-particle states plays a key role for the stability of the Higgs mode discussed below. \( |\varepsilon_{kk'}\rangle = |\downarrow\rangle_k \bigotimes \prod_{k_F} |\uparrow\rangle \bigotimes |\varepsilon_{kk'}\rangle \) (\( l = 0, 0 \)) are degenerate single-particle states with excitation energy \( 2E_k \) that form the two-particle continuum. They have even \((l = 0)\) and odd \((l = 0)\) parity under \( C_{kk'} \). They both have even parity under \( C_{kF} \). \( |\varepsilon_{kk'}\rangle = |\downarrow\rangle_k \bigotimes \prod_{k_F} |\uparrow\rangle \bigotimes \prod_{k_F} |\uparrow\rangle \bigotimes \prod_{k_F} |\downarrow\rangle \). The Higgs mode is uncoupled with the single-particle states because \( |\varepsilon_{kk'}\rangle \). Thus, the Higgs mode is a stable excitation of \( \mathcal{H}_I \).

**Strong-coupling perturbation theory.**—Having shown the emergence of the Higgs mode due to breakdown of \( Z_2 \) in the weak-coupling theory, we demonstrate it as well in a strong-coupling approach, where we treat \( \mathcal{H}_K \) as a perturbation to the unperturbed Hamiltonian \( \mathcal{H}_X \). It is valid when \( N g \) is much larger than the band width, i.e., \( N g \gg \max |\xi_k| \), where \( N \) is the total number of wave vectors. Given that the Higgs mode has even parity for all \( C_{kk'} \), we treat \( S'_{\mu kk} \) as a spin-1 operator to take into account only even parity states under \( C_{kk'} \).

Each eigenstate of \( \mathcal{H}_{MF} \) has a corresponding eigenstate
The degeneracy among the first-excited states \( \{ |0_k \} \) is lifted by diagonalizing the second-order effective Hamiltonian \( \mathcal{H}_{\text{eff}} \equiv \mathcal{H}(E_{0k}^0 - \mathcal{H}_X)^{-1} \mathcal{H}_K \), where \( E_{0k}^0 \equiv (N - 1)g \) is the unperturbed energy of \( |0_k \)\). The effective Hamiltonian can be written as

\[
\mathcal{H}_{\text{eff}} = \sum_k J_k |0_k\rangle \langle 0_k| - \sum_{k \neq k'} J_{k,k'} |0_k\rangle \langle 0_{k'}| ,
\]

where

\[
J_k = \frac{2 \xi_k^2}{(N - 1)g} , \quad J_{k,k'} = \frac{4 \xi_k \xi_{k'}}{(N - 1)(N - 3)g} .
\]

Note that energy in Eq. (15) is measured from \( E_{0k}^0 - \Delta E_{kF} \), where \( \Delta E_{kF} = \frac{2 \sum_n \xi_n^2}{(N - 3)g} \) is the second-order energy shift of \( \sigma_{zF} \langle G \rangle \) that corresponds to \( |e_{kF} \rangle \). The first term in Eq. (15) represents the energy continuum above the threshold \( E_{0k}^0 - \Delta E_{kF} \), as shown in Fig. 2.

We consider the following state:

\[
|\Phi\rangle = \sum_k \frac{1}{\xi_k} |0_k\rangle .
\]

Using Eq. (15), we obtain

\[
\mathcal{H}_{\text{eff}} |\Phi\rangle = \sum_k C_k |0_k\rangle , \quad C_k = \frac{J_k}{\xi_k} + \sum_{k' \neq k} \left( -\frac{J_{k,k'}}{\xi_{k'}} \right) .
\]

In the limit \( N \gg N_{kF} \), using \( \sum_{k' \neq k} 1 \approx N/2 \), Eq. (15) reduces to \( \mathcal{H}_{\text{eff}} |\Phi\rangle = 0 \). Remarkably, \( |\Phi\rangle \) represents a bound state of \( \{ |0_k\rangle \} \) that is formed at the lower edge of the energy continuum at \( 2\Delta_0 \). On the other hand, we find \( \beta_{11}^0 |\Psi\rangle \rightarrow |\Phi\rangle \) in the strong-coupling limit using \( \beta_{11}^0 \rightarrow -i \sum_{k'} (S_{kk'} - i S_{zkk'})/\xi_k \). Thus, the Higgs mode \( |\Phi\rangle \) arises in the strong-coupling theory. \( |\Phi\rangle \) is indeed stable, because it is uncoupled with \( \sigma_{zF} \langle G \rangle \). In the weak-coupling regime, since \( |0_k\rangle \) corresponds to \( |e_{kF}^0 \rangle \), \( \beta_{11}^0 |\Psi\rangle \) is considered a bound state of \( \{ |0_{kF}^0 \rangle \} \) formed at \( 2\Delta_0 \).

**Multiple Higgs modes.** We expect that a bound state analogous to the Higgs mode may be formed among the first excited states in each block. The effective Hamiltonian \( \mathcal{H}_{\text{eff}}^{(n)} \) for the degenerate first excited states \( \{ Z(\{ k_F \}) |0_k \} \) in the block of \( Z(\{ k_F \}) \) \( \mathcal{G} \) is given by

\[
\mathcal{H}_{\text{eff}}^{(n)} = \sum_k J_k^{(n)} Z \langle 0_k | Z - \sum_{k \neq k'} J_{k,k'}^{(n)} Z \langle 0_k | Z (19)
\]

where

\[
J_k^{(n)} = \frac{2 \xi_k^2}{(N - 2n + 1)g} ,
\]

\[
J_{k,k'}^{(n)} = \frac{4 \xi_k \xi_{k'}}{(N - 2n + 1)(N - 2n + 3)g} .
\]

Here, \( n \) is the number of wave vectors in \( \{ k_F \} \). In the limit \( N \gg N_{kF} \), we find that \( \mathcal{H}_{\text{eff}}^{(n)} \) has a Higgs-like bound state

\[
|\Phi^{(n)}\rangle = Z(\{ k_F \}) |\Phi\rangle .
\]

Thus, combining with the original Higgs mode \( |\Phi^{(0)}\rangle \equiv |\Phi\rangle \), the multiple Higgs modes \( |\Phi^{(n)}\rangle (0 \leq n \leq N_{kF}) \) have quantized energy \( 2(n+1)\Delta_0 \). They have odd parity.
under $C_{k_F}$ for $n$ Fermi wavevectors in $\{k_F\}$. They should appear in the weak-coupling regime. They correspond to the states $\mathcal{Z}(\{k_F\})\beta_H^0(\Psi)$ with quantized energy $2(n + 1)\Delta_0$ in the weak-coupling regime.

These multiple Higgs modes may be observable in superconductors with CDW-order such as NbSe$_2$ using Raman spectroscopy\cite{14}. Their signature may appear as multiple resonance peaks at frequencies $2(n + 1)\Delta_0$ in Raman spectrum. It may be also possible to observe them using recently developed terahertz spectroscopy techniques\cite{10}.

Conclusions and conjectures.— We have shown that the Higgs mode emerges due to spontaneous breakdown of $Z_2$ under $T$ in a superconductor. We further predicted the existence of the multiple Higgs modes that have quantized energy $2(n + 1)\Delta_0$ ($0 \leq n \leq N_{k_F}$).

The analysis in the present work has broad applicability in condensed-matter and particle physics. Multiple Higgs modes may appear in systems for which the BCS theory is applicable, such as fermionic superfluids, atomic nuclei, and quark matters. It would be reasonable to conjecture that Higgs modes in other condensed-matter systems, such as a bosonic superfluid in an optical lattice and quantum spin systems, also arise due to spontaneous breakdown of $Z_2$ symmetries. Extensions of the present work to these systems are left for the future.

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* Electronic address: tsuchiya@phys.chuo-u.ac.jp

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Supplemental Materials

Pseudospin Operators

In this Section, we summarize the algebra for the pseudospin operators. We introduce $S_{\mu \nu \rho}^{kk}$ in Eq. (9) in the main text. We also introduce another pseudospin operator $\tilde{S}_{\mu \nu \rho}^{kk}$ as

$$\tilde{S}_{\mu \nu \rho}^{kk} = S_{\mu \nu \rho}^{kk} + (-1)^{\delta_{\mu \nu}} S_{\rho \mu \nu}^{kk}, \quad (\mu = x, y, z),$$

(23)

where $k$ is above the Fermi surface (FS) ($\xi_k > 0$). $S_k$ is transformed by $C_{kk'}$ and $C_{kk'}$ as

$$C_{kk'} S_{\mu \nu \rho}^{kk} C_{kk'} = \begin{cases} (-1)^{\delta_{\mu \nu}} S_{\rho \mu \nu}^{kk'} & \text{if } k' = k, k, \\ S_{\rho \mu \nu}^{kk'} & \text{otherwise,} \end{cases}$$

(24)

$$C_{kk'} S_{\mu \nu \rho}^{kk} C_{kk'} = \begin{cases} (-1)^{\delta_{\mu \nu}} S_{\rho \mu \nu}^{kk} & \text{if } k = k, k, \\ S_{\rho \mu \nu}^{kk} & \text{otherwise.} \end{cases}$$

(25)

Using Eqs. (24) and (25), one can derive the commutation relations

$$[C_{kk'}, S_{\mu \nu \rho}^{kk}] = [S_{\mu \nu \rho}^{kk}, \tilde{S}_{\mu \nu \rho}^{kk}] = 0.$$  

(26)

$S_{kk}$ and $\tilde{S}_{kk}$ also satisfy

$$[S_{\mu \nu \rho}^{kk}, S_{\sigma \tau \delta}^{kk}] = [\tilde{S}_{\mu \nu \rho}^{kk}, \tilde{S}_{\sigma \tau \delta}^{kk}] = i \sum_{\rho} \tilde{\omega}_{\mu \nu \rho} S_{\rho \mu \nu}^{kk'},$$

(27)

$$[S_{\mu \nu \rho}^{kk}, \tilde{S}_{\sigma \tau \delta}^{kk}] = i \sum_{\rho} \tilde{\omega}_{\mu \nu \rho} \tilde{S}_{\rho \mu \nu}^{kk'},$$

(28)

$S_{\mu \nu \rho}^{kk} S_{\sigma \tau \delta}^{kk} = S_{\mu \nu \rho}^{kk} S_{\sigma \tau \delta}^{kk} = 0$, $S_{\mu \nu \rho}^{kk} S_{\sigma \tau \delta}^{kk} = S_{\mu \nu \rho}^{kk} S_{\sigma \tau \delta}^{kk} = 1.$

(29)

The spin-1 triplet states for $S_{\mu \nu \rho}^{kk}$ can be written as

$$|1\rangle_{kk} = |\uparrow\rangle_{kk},$$

(30)

$$|0\rangle_{kk} = \frac{1}{\sqrt{2}} (|\uparrow\rangle_{kk} + |\downarrow\rangle_{kk}),$$

(31)

$$|-1\rangle_{kk} = |\downarrow\rangle_{kk},$$

(32)

Here, we denote $|s\rangle_{kk} = |s\rangle_{kk} \otimes |t\rangle_{kk}$ $(s, t = \uparrow, \downarrow)$. They satisfy $S_{\mu \nu \rho}^{kk} |m\rangle_{kk} = m |m\rangle_{kk}$ $(m = 1, 0, -1)$ and have even parity under $C_{kk'}$: $C_{kk'} |m\rangle_{kk} = |m\rangle_{kk}$.

The spin-1 triplet states for $S_{\mu \nu \rho}^{kk}$ can be written as

$$|1\rangle_{kk} = |\uparrow\rangle_{kk},$$

(33)

$$|0\rangle_{kk} = \frac{1}{\sqrt{2}} (|\uparrow\rangle_{kk} + |\downarrow\rangle_{kk}),$$

(34)

$$|-1\rangle_{kk} = |\downarrow\rangle_{kk},$$

(35)

where $|\pm\rangle_k = (|\uparrow\rangle_k \pm i |\downarrow\rangle_k) / \sqrt{2}$. They satisfy $S_{\mu \nu \rho}^{kk} |m\rangle_{kk} = m |m\rangle_{kk}$ $(m = 1, 0, -1)$ and have even parity under $C_{kk'}$: $C_{kk'} |m\rangle_{kk} = |m\rangle_{kk}$.

The spin-0 singlet state $|0\rangle_{kk}$ can be written as

$$|0\rangle_{kk} = \frac{1}{\sqrt{2}} (|\uparrow\rangle_{kk} + |\downarrow\rangle_{kk}.$$

(36)

It satisfies $S_{\mu \nu \rho}^{kk} |0\rangle_{kk} = 0$ $(\mu = x, y, z)$ and has odd parity under $C_{kk'}$: $C_{kk'} |0\rangle_{kk} = - |0\rangle_{kk}$. We note that the pseudospins for $k$ and $\tilde{k}$ are entangled in $|0\rangle_{kk}$, $|0\rangle_{kk}$, and $|0\rangle_{kk}$.

$S_{\mu \nu \rho}^{kk} = S_{\mu \nu \rho}^{kk} + i S_{\mu \nu \rho}^{kk}$ are the ladder operators for the spin-1 triplet states $\{ |m\rangle_{kk} \}$:

$$S_{\mu \nu \rho}^{kk} |1\rangle_{kk} = S_{\mu \nu \rho}^{kk} |1\rangle_{kk} = \sqrt{2} |0\rangle_{kk},$$

(38)

$$S_{\mu \nu \rho}^{kk} |1\rangle_{kk} = S_{\mu \nu \rho}^{kk} |1\rangle_{kk} = 0,$$

(39)

$$S_{\mu \nu \rho}^{kk} |0\rangle_{kk} = \sqrt{2} |1\rangle_{kk},$$

(40)

$$S_{\mu \nu \rho}^{kk} |0\rangle_{kk} = \sqrt{2} |1\rangle_{kk}.$$

(41)

$$S_{\mu \nu \rho}^{kk} |0\rangle_{kk} = \sqrt{2} |1\rangle_{kk}.$$

(42)

$$S_{\mu \nu \rho}^{kk} |0\rangle_{kk} = \sqrt{2} |1\rangle_{kk}.$$

(43)

In general, operating $S_{\mu \nu \rho}^{kk}$ on a certain state changes its parity under $C_{kk'}$, while operating $S_{\mu \nu \rho}^{kk}$ does not as

$$C_{kk'} S_{\mu \nu \rho}^{kk} |\psi_{e(o)}\rangle_{kk} = \pm S_{\mu \nu \rho}^{kk} |\psi_{e(o)}\rangle_{kk},$$

(45)

$$C_{kk'} S_{\mu \nu \rho}^{kk} |\psi_{e(o)}\rangle_{kk} = \mp S_{\mu \nu \rho}^{kk} |\psi_{e(o)}\rangle_{kk},$$

(46)

where $|\psi_{e(o)}\rangle_{kk}$ denotes an even (odd) parity state under $C_{kk'}$. The upper (lower) signs on the right-hand-sides of Eqs. (45) and (46) are for the even (odd) parity state.
Applications of Pseudospin Operators

In this Section, for illustration of applications of the pseudospin operators introduced in the previous Section, we describe the normal state in terms of them and also derive some rigorous relations for occupation numbers of fermions and dynamical spin susceptibilities.

We first consider the normal state. Given the kinetic energy term in Eq. (10), the ground state of $\mathcal{H}_K$ can be written as $|\Psi_0\rangle = \prod_k (|k\rangle \otimes |\Phi_F\rangle)$, where $|\Phi_F\rangle$ denotes the wave function for the pseudospins on the FS, which are zero modes for $\mathcal{H}_K$. Using Eqs. (27) and (28), we obtain

$$ [\mathcal{H}_K, S_{k\sigma}^\pm] = \pm 2\xi_k S_{k\sigma}^\pm , \quad (47) $$

$$ [\mathcal{H}_K, \tilde{S}_{k\sigma}^\pm] = \pm 2\xi_k \tilde{S}_{k\sigma}^\pm . \quad (48) $$

The above equations show that $S_{k\sigma}^\pm$ and $\tilde{S}_{k\sigma}^\pm$ are the raising and lowering operators for the eigenstates of $\mathcal{H}_K$. Thus, $S_{k\sigma}^\pm |\Psi_0\rangle / \sqrt{2}$ and $\tilde{S}_{k\sigma}^\pm |\Psi_0\rangle / \sqrt{2}$ are the degenerate excited states with excitation energy $2\xi_k$ involving a pair of fermions, where they have even and odd parity under $C_{k\sigma}$, respectively.

We derive the fermion occupation number for $|\psi_{e(0)}\rangle_{k\bar{k}}$. Using Eq. (49), we obtain

$$ k\bar{k} \langle \psi_{e(0)} | \tilde{S}_{k\bar{k}} \psi_{e(0)} \rangle_{k\bar{k}} = 0 . \quad (49) $$

Specifically, from the $z$-component of Eq. (49) we obtain the quantization of fermion occupation number

$$ k\bar{k} \langle \psi_{e(0)} | (n_{k\uparrow} + n_{k\downarrow} + n_{\bar{k}\uparrow} + n_{\bar{k}\downarrow}) \psi_{e(0)} \rangle_{k\bar{k}} = 2 , \quad (50) $$

where $n_{k\sigma} = c_{k\sigma}^\dagger c_{k\sigma}$ is the fermion number operator. We also obtain

$$ k\bar{k} \langle \uparrow \rangle_{k\bar{k}} \langle \downarrow \rangle_{k\bar{k}} = (1/2, 0, 0) , \quad (51) $$

where $\langle \uparrow \rangle_{k\bar{k}} (\langle \downarrow \rangle_{k\bar{k}})$ is an even (odd) parity state under $C_{k\sigma}$. The upper (lower) sign on the right-hand-side of Eq. (51) is for $\langle \uparrow \rangle_{k\bar{k}} (\langle \downarrow \rangle_{k\bar{k}})$. From the $z$-component of Eq. (51), we obtain

$$ k\bar{k} \langle \uparrow \rangle (n_{k\uparrow} + n_{\bar{k}\downarrow}) \langle \downarrow \rangle_{k\bar{k}} = 1 . \quad (52) $$

Therefore, the states $|\psi_{e(0)}\rangle_{k\bar{k}}$ and $|\uparrow\rangle_{k\bar{k}}$ that appear in the eigenstates of $\mathcal{H}_f$ are half-filled.

One can also derive some rigorous relations for the dynamical spin susceptibility

$$ \chi_{\mu k, \nu}(\omega) = -i \int_0^\infty \langle [S_{\mu k}(t), S_{\nu k}(t)] \rangle e^{-i\omega t} dt , \quad (53) $$

where $S_{\mu k}(t) = e^{-i\mathcal{H}_f t} S_{\mu k} e^{i\mathcal{H}_f t}$ is the Heisenberg representation and $\langle \cdots \rangle$ denotes the thermal average. We focus on $\chi_{y k, x}(\omega)$ and evaluate

$$ \langle [S_{y k}(t), S_{y k}(t)] \rangle \propto \sum_n e^{-\beta E_n} \langle n | [S_{x k}, S_{y k}(t)] | n \rangle , \quad (54) $$

where $\beta$ is the inverse temperature and $|n\rangle$ denotes an eigenstate of $\mathcal{H}_f$: $\mathcal{H}_f |n\rangle = E_n |n\rangle$. Since operating $\tilde{S}_{y k\bar{k}}$ changes the parity of the state under $C_{k\bar{k}}$, we obtain $\langle n | \tilde{S}_{y k\bar{k}}(t) | n \rangle = \langle n | \tilde{S}_{y k\bar{k}}(t) \tilde{S}_{y k\bar{k}}(t) | n \rangle = 0$ and therefore $\langle n | S_{x k} \tilde{S}_{y k\bar{k}}(t) | n \rangle = -\langle n | S_{x k} \tilde{S}_{y k\bar{k}}(t) | n \rangle$ and $\langle n | S_{y k\bar{k}}(t) S_{x k} | n \rangle = -\langle n | S_{y k\bar{k}}(t) S_{x k} | n \rangle$. On the other hand, one can also derive $\langle n | S_{y k} S_{y k\bar{k}}(t) | n \rangle = 0$ using $C_{k\bar{k}} S_{y k\bar{k}}(t) C_{k\bar{k}} = -S_{y k\bar{k}}(t)$. We thus obtain

$$ \chi_{y k, x}(\omega) = -\chi_{y k, x}(\omega) , \quad (55) $$

$$ \chi_{x k, y}(\omega) = 0 . \quad (56) $$

Equations (55) and (56) lead to the out-of-phase oscillations of spin fluctuations for the Higgs mode $\delta S_{y k\bar{k}} = -\delta S_{y k\bar{k}}$ in the classical spin analysis [42]. Analogously, one can show

$$ \chi_{x k, y}(\omega) = -\chi_{x k, y}(\omega) , \quad (57) $$

$$ \chi_{x k, y}(\omega) = 0 . \quad (58) $$

using $\langle n | \tilde{S}_{y k\bar{k}}(t) \tilde{S}_{k\bar{k}}(t) | n \rangle = \langle n | S_{y k\bar{k}}(t) S_{y k\bar{k}}(t) | n \rangle = 0$, $\langle n | S_{y k\bar{k}}(t) S_{y k\bar{k}}(t) | n \rangle = \langle n | S_{y k\bar{k}}(t) S_{y k\bar{k}}(t) | n \rangle = 0$, and $\langle n | S_{y k\bar{k}}(t) S_{y k\bar{k}}(t) | n \rangle = \langle n | S_{y k\bar{k}}(t) S_{y k\bar{k}}(t) | n \rangle = 0$. We thus find that the dynamical spin susceptibilities for total spin vanish as $\chi_{y y}(\omega) = \sum_{k\bar{k}} \chi_{x k, y}(\omega) = 0$ and $\chi_{x y}(\omega) = \sum_{k\bar{k}} \chi_{x k, y}(\omega) = 0$ [42]. The expressions for the MF theory

$$ \chi_{y k, x}(\omega) \propto \frac{\omega \xi_k}{E_k(4E_k^2 - \omega^2)} , \quad (59) $$

indeed satisfy Eqs. (55)~(58) [42].

Pseudospin Operators for Bogolons

In this Section, we summarize the algebra for the pseudospin operators for bogolons. $S'_k$ is introduced as [42]

$$ \begin{pmatrix} S'_{x k} \\ S'_{y k} \end{pmatrix} = \begin{pmatrix} -\cos \varphi_k & -\sin \varphi_k \\ \sin \varphi_k & -\cos \varphi_k \end{pmatrix} \begin{pmatrix} z_{x k} \\ z_{y k} \end{pmatrix} , \quad (60) $$

where $\cos \varphi_k = -\xi_k / E_k$ and $\sin \varphi_k = \Delta_0 / E_k$. $S'_k$ is rotated about the angle $\pi - \varphi_k$ in the $x$-$z$ plane in Eq. (50). Using Eq. (60), the MF Hamiltonian can be written in the form of Eq. (11). The eigenstates of $S'_{x k}$ are given as

$$ | \uparrow \rangle_k = u_k | \uparrow \rangle_k - v_k | \downarrow \rangle_k , \quad (61) $$

$$ | \downarrow \rangle_k = u_k | \downarrow \rangle_k + v_k | \uparrow \rangle_k , \quad (62) $$

where $| \uparrow \rangle_k$ represents the vacuum of bogolons and $| \uparrow \rangle_k$ the excited state with a pair of bogolons. All the pseudospins $S'_k$ are aligned downward in the $z$ direction in the superconducting (SC) ground state. The BCS wave function can be thus written as

$$ |\Psi\rangle = \prod_k | \downarrow \rangle_k . \quad (63) $$
Note that \((S'_x k_F, S'_y k_F, S'_z k_F) = (S_z k_F, S_y k_F, -S_z k_F), |\uparrow k_F\rangle = |\uparrow k_F\rangle\), and \(|\downarrow k_F\rangle = |\downarrow k_F\rangle\).

We introduce another pseudospin operator \(\tilde{S}_{k_F}^I\) as \(\tilde{S}_{k_F}^I = S'_x + (1)^{\delta_{y<0}} S'_y, \ (\mu = x, y, z), \) where \(k_F\) is above the FS \((\xi_{k_F} > 0)\). \(S'_k\) is transformed by \(C_k\) and \(C_{k_F}\) as \(C_k S'_k C_{k_F} = \left\{ \begin{array}{ll} (1)^{\delta_{y<0}} S'_k, & \text{otherwise,} \\
\end{array} \right. \)

\(C_{k_F} S'_k C_{k_F} = \left\{ \begin{array}{ll} (1)^{\delta_{y<0}} S'_k, & \text{otherwise,} \\
\end{array} \right. \)

Using Eqs. \((65)\), one can derive the commutation relations \(\{C_{k_F}, S'_k\} = 0\).

The spin-1 triplet states \(S'_{k_F}\) can be written as \(|\uparrow k_F\rangle = (|\uparrow k_F\rangle \pm |\downarrow k_F\rangle) / \sqrt{2}\),\n
\(|0 k_F\rangle = \frac{1}{\sqrt{2}} (|\uparrow k_F\rangle - |\downarrow k_F\rangle)\),\n
\(|-1 k_F\rangle = (|\uparrow k_F\rangle + |\downarrow k_F\rangle) / \sqrt{2}\).

They satisfy \(S'_x |m' k_F\rangle = m |m' k_F\rangle (m = 1, 0, -1)\). They have even parity under \(C_k\); \(|m' k_F\rangle = |m' k_F\rangle\). The spin-0 singlet state \(|0 k_F\rangle\) is given as \(|0 k_F\rangle = \frac{1}{\sqrt{2}} (|\uparrow k_F\rangle + |\downarrow k_F\rangle)\).

Given the MF Hamiltonian in Eq. \((11)\), using Eqs. \((68)\) and \((69)\), one obtains \(\[ H_{MF}, S'_{k_F}^+ \] = \pm 2E_k S'_{k_F}, \)

\(\[ H_{MF}, \tilde{S}_{k_F}^+ \] = \pm 2E_k \tilde{S}_{k_F}^+ \), \(\[ H_{MF}, S'_{k_F}^- \] = \pm 2D_0 S'_{k_F}^- \).

\(S'_{k_F}^+\) and \(S'_{k_F}^\pm\) are the raising and lowering operators for the eigenstates of \(H_{MF}\). \(|e_{k_F}\rangle = S'_{k_F}^\pm |\Psi\rangle / \sqrt{2}\) are the degenerate excited states with excitation energy \(2E_k\) that involves a single pair of bosons. They have even and odd parity under \(C_{k_F}\), respectively. \(|e_{k_F}\rangle = S'_{k_F}^\pm |\Psi\rangle (79)\) is an excited state with excitation energy \(2\Delta_0\)

**Holstein-Primakoff Theory applied to \(H_I\)**

In this Section, we apply the Holstein-Primakoff theory to \(H_I\) in order to derive the Higgs mode. Substituting Eq. \((66)\) into \(H_I\), it can be written as

\(H_I = \sum_k 2\zeta_k (-\cos \varphi_k S'_{z k_F} + \sin \varphi_k S'_{y k_F}) - g \left\{ \sum_{k, k'} (\cos \varphi_k \cos \varphi_{k'} S'_{x k_F} S'_{x k'_F} + \sin \varphi_k \cos \varphi_{k'} S'_{y k_F} S'_{y k'_F} + \sin \varphi_k \sin \varphi_{k'} S'_{z k_F} S'_{z k'_F}) + 2 \sum_{k_F} (\sin \varphi_k S'_{y k_F} - \cos \varphi_k S'_{x k_F}) S_{z k_F} \right\} + \sum_{k_F, k'} S_{z k_F} S_{z k'_F} \) (84)

Since the eigenstates of \(H_I\) can be characterized by the parity under \(C_{k_F}\), we can treat \(S_{z k_F}\) as a \(\epsilon\)-number. \(S_{x k_F} = \pm 1 / 2\). We quantize spin fluctuations around the ground state \(|\Psi\rangle\) by the Holstein-Primakoff transformation \([45]\):

\(S'_{z k_F} = \sqrt{2S} \gamma_{k_F} \sqrt{1 - \frac{\gamma_{k_F}^* \gamma_{k_F}}{2S}}, \ S'_{k_F} = (S'_{k_F})^\dagger, \) \(S'_{k_F} = \left\{ \begin{array}{ll} (1)^{\delta_{y<0}} S'_{k_F}, & \text{otherwise,} \\
\end{array} \right. \)

where \(\gamma_{k_F}\) and \(\gamma_{k_F}\) denote, respectively, the creation and annihilation operators of a boson that represents spin fluctuations. They satisfy the usual commutation relations \(|\gamma_{k}, \gamma_{k'}\rangle = \delta_{k, k'}\) and \(|\gamma_{k}, \gamma_{k'}\rangle = [\gamma_{k}, \gamma_{k'}] = 0\). In view of the fact that the creation operator of the Higgs mode derived from \(H_{BCS}\) in Ref. \([42]\) has even parity under \(C_{k_F}\), we restrict the Hilbert space spanned by even-parity states under \(C_{k_F}\), in which \(S_{k_F}\) represents a spin-1
operator. We thus set $S = 1$. If spin fluctuation is small ($\gamma_k \gamma_k \ll 1$), $S_{\kappa \kappa}^\pm$ can be approximated as $S_{\kappa \kappa}^\pm \simeq \sqrt{2} \gamma_k^\dagger$ and $S_{\kappa \kappa}^\dagger \simeq \sqrt{2} \gamma_k$.

We expand Eq. (83) in terms of $\gamma_k$ and $\gamma_k^\dagger$. The zeroth and first-order terms read

$$H_i^{(0)} = -2 \sum_k \frac{\xi_k^2}{E_k} \Delta_0^2 - \frac{\Delta_0^2}{g} ,$$  

$$H_i^{(1)} = \sqrt{2} \sum_k (\xi_k \sin \varphi_k + \Delta_0 \cos \varphi_k)(\gamma_k + \gamma_k^\dagger) .$$  

(87)

(88)

Here, we have used the approximation

$$\Delta_0 = g(\sum_k \sin \varphi_k + \sum_{k \neq k'} S_{\kappa k'}) \simeq g(\sum_k \sin \varphi_k) .$$  

(89)

Since $H_i^{(1)}$ should vanish, we obtain $\sin \varphi_k = \Delta_0 / E_k$ and $\cos \varphi_k = -\xi_k / E_k$. Equation (89) thus reduces to the gap equation

$$1 = g \sum_k \frac{1}{E_k} .$$  

(90)

The second-order term reads

$$H_i^{(2)} = 2 \sum_k E_k \gamma_k^\dagger \gamma_k \frac{g}{2} \sum_{k \neq k'} \cos \varphi_k \cos \varphi_{k'} \times (\gamma_k \gamma_{k'}^\dagger + \gamma_k^\dagger \gamma_{k'} + \gamma_k \gamma_{k'} + \gamma_k^\dagger \gamma_{k'}^\dagger) .$$  

(91)

We diagonalize $H_i^{(2)}$ by the Bogoliubov transformation

$$\beta_\lambda = \sum_k (U_{\lambda k}^* \alpha_k^\dagger + V_{\lambda k}^* \alpha_k) ,$$  

$$\beta_\lambda^\dagger = \sum_k (U_{\lambda k} \alpha_k^\dagger + V_{\lambda k} \alpha_k) ,$$  

(92)

(93)

where $\lambda$ labels the normal modes. The bosonic operator $\beta_\lambda$ satisfies the commutation relations

$$[\beta_\lambda, \beta_\lambda^\dagger] = \sum_k (U_{\lambda k}^* U_{\lambda' k'} - V_{\lambda k}^* V_{\lambda' k'}) = \delta_{\lambda \lambda'} ,$$  

$$[\beta_\lambda^\dagger, \beta_\lambda] = \sum_k (-U_{\lambda k} V_{\lambda k}^* + V_{\lambda k}^* U_{\lambda k}) = 0 .$$  

(94)

(95)

One can derive the inverse transformation from Eqs. (92) and (93) as

$$\gamma_k = \sum_\lambda (U_{\lambda k} \beta_\lambda - V_{\lambda k} \beta_\lambda^\dagger) ,$$  

$$\gamma_k^\dagger = \sum_\lambda (U_{\lambda k}^* \beta_\lambda^\dagger + V_{\lambda k}^* \beta_\lambda) .$$  

(96)

(97)

Assuming that the second order term is diagonalized as $H_i^{(2)} = \sum_\lambda \omega_\lambda \beta_\lambda^\dagger \beta_\lambda + \text{const.}$, we obtain

$$[\gamma_k, H_i^{(2)}] = \sum_\lambda \omega_\lambda (U_{\lambda k} \beta_\lambda + V_{\lambda k} \beta_\lambda^\dagger) .$$  

(98)

On the other hand, using Eq. (91), we obtain

$$[\gamma_k, H_i^{(2)}] = \sum_\lambda \left\{ \left( 2 E_k U_{\lambda k} - g \sum_{k'}' \cos \varphi_k \cos \varphi_{k'} (U_{\lambda k'}^* - V_{\lambda k'}) \right) \beta_\lambda + \left( -2 E_k V_{\lambda k} - g \sum_{k'}' \cos \varphi_k \cos \varphi_{k'} (U_{\lambda k'}^* - V_{\lambda k'}) \right) \beta_\lambda^\dagger \right\} .$$  

(99)

For Eqs. (98) and (99) to be consistent, $X_{\lambda k}$ and $Y_{\lambda k}$ should satisfy

$$2 E_k U_{\lambda k} - g (e_\lambda - f_\lambda) \cos \varphi_k = \omega_\lambda U_{\lambda k} \ ,$$  

$$-2 E_k V_{\lambda k} - g (e_\lambda - f_\lambda) \cos \varphi_k = \omega_\lambda V_{\lambda k} \ ,$$  

(100)

(101)

where the coefficients $e_\lambda$ and $f_\lambda$ are given by

$$e_\lambda = \sum_k' \cos \varphi_k U_{\lambda k} ,$$  

$$f_\lambda = \sum_k' \cos \varphi_k V_{\lambda k} .$$  

(102)

(103)

If $e_\lambda - f_\lambda \neq 0$, Eqs. (100) and (101) can be formally solved as

$$U_{\lambda k} = \frac{g (e_\lambda - f_\lambda) \cos \varphi_k}{2 E_k - \omega_\lambda} \ ,$$  

$$V_{\lambda k} = -\frac{g (e_\lambda - f_\lambda) \cos \varphi_k}{2 E_k + \omega_\lambda} .$$  

(104)

(105)

We omit $\lambda$ below.

Substituting Eqs. (104) and (105) into Eqs. (102) and (103), we obtain

$$1 - 4 g \sum_k \frac{\xi_k^2}{E_k} \frac{E_k}{4 E_k^2 - \omega^2} = 0 .$$  

(106)

The above equation has a solution $\omega = 2 \Delta_0$, for which it reduces to the MF gap equation (90). We thus obtain

$$U_k = \frac{B \cos \varphi_k}{2 \Delta_0 - 2 E_k} \ ,$$  

$$V_k = \frac{B \cos \varphi_k}{2 \Delta_0 + 2 E_k} ,$$  

(107)

where $B$ is the normalization constant. $B$ is determined by the normalization condition (94) as

$$B = \frac{1}{\sqrt{\sum_k \xi_k^2 / E_k} \Delta_0} .$$  

(108)

The creation operator for the collective excitation with $\omega = 2 \Delta_0$ is thus given by

$$\beta_\lambda^\dagger = B \sum_k \frac{\xi_k}{E_k} \left( \frac{\gamma_k^\dagger}{2 \Delta_0 - 2 E_k} + \frac{\gamma_k}{2 \Delta_0 + 2 E_k} \right) .$$  

(109)

$\beta_\lambda^\dagger$ coincides with the creation operator of the Higgs mode derived from $H_{BCS}$ (See Eq. (C31) in Ref. [42]).
using $\alpha_k^\dagger - \alpha_k = \sqrt{2}\gamma_k$. Here, $\alpha_k$ is a creation operator of a boson that describes fluctuations of the spin-1/2 operator $S'_k$ (see Eqs. (C2) and (C3) in Ref. [42]).

In the limit of small fluctuations ($\gamma_k \gamma_k \ll 1$), using $\gamma_k^\dagger \approx S'_{kk}^+/\sqrt{2}$ and $\gamma_k \approx S'_{kk}^-/\sqrt{2}$, the creation operator for the Higgs mode can be written as

$$\beta_H^\dagger = \frac{B}{\sqrt{2}} \sum_k \xi_k \left( \frac{S'_{kk}^+}{2\Delta_0 - 2E_k} + \frac{S'_{kk}^-}{2\Delta_0 + 2E_k} \right).$$

(110)

We omit the normalization constant in Eq. (13) in the main text. The excited state with a single Higgs mode can be written in terms of $|\phi_{kk}\rangle$ as

$$\beta_H^\dagger |\Psi\rangle = B \sum_k \frac{\xi_k}{E_k} \frac{1}{2\Delta_0 - 2E_k} |\phi_{kk}\rangle.$$  

(111)