Majorana Fermions in Self-Consistent Effective Hamiltonian Theory

Xindong Wang[1, *]
[1] *Sophyics Technology, LLC, McLean, VA 22102, USA*
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Majorana fermion solution is obtained from the self-consistent effective Hamiltonian theory[1]. The ground state is conjectured to be a non-empty vacuum with 2 fermions, one for each type. The first type is the original charged fermion and the second type the chiral charge-less Majorana fermion. The Marjorana fermion is like a shadow of the first fermion cast by the non-empty vacuum.

Recently, Wang et. al.[1] apply the Bogolyubov transformation to the 4 local many-body basis states and conjectured that for ground state, due to Pauli exclusion principle, only 3-local basis is needed and further derived a tight-binding version of the quadratic Hamiltonian. In this letter, we formulate a similar variational Ansatz in the continuum limit and solves the two chiral-symmetry broken modes for fermionic excitations. We begin with the following variational Ansatz:
For any spin-1/2 fermionic ground state, there exist an effective vacuum field $|\text{Vac}(\boldsymbol{x})\rangle$, defined by the unitary Bogolyubov transformation related to $\{\alpha(\boldsymbol{x}), \beta(\boldsymbol{x})\}$:

$$\begin{pmatrix} \hat{\xi}_\uparrow(\boldsymbol{x}) \\ \hat{\xi}_\downarrow(\boldsymbol{x}) \\ \hat{\xi}^\dagger_\downarrow(\boldsymbol{x}) \\ \hat{\xi}^\dagger_\uparrow(\boldsymbol{x}) \end{pmatrix} = \begin{pmatrix} -\alpha(\boldsymbol{x}) & 0 & \beta(\boldsymbol{x}) & 0 \\ 0 & \beta^*(\boldsymbol{x}) & 0 & \alpha^*(\boldsymbol{x}) \\ \beta(\boldsymbol{x}) & 0 & \alpha(\boldsymbol{x}) & 0 \\ 0 & -\alpha^*(\boldsymbol{x}) & 0 & \beta^*(\boldsymbol{x}) \end{pmatrix} \begin{pmatrix} \hat{\psi}_\uparrow(\boldsymbol{x}) \\ \hat{\psi}_\downarrow(\boldsymbol{x}) \\ \hat{\psi}^\dagger_\downarrow(\boldsymbol{x}) \\ \hat{\psi}^\dagger_\uparrow(\boldsymbol{x}) \end{pmatrix} \tag{1}$$

and

$$\begin{aligned} \hat{\xi}_\sigma(\boldsymbol{x})|\text{Vac}(\boldsymbol{x})\rangle =& 0 \\ |\text{Vac}(\boldsymbol{x})\rangle =& \alpha(\boldsymbol{x})|0\rangle + \beta(\boldsymbol{x})\hat{\psi}^\dagger_\uparrow(\boldsymbol{x})\hat{\psi}^\dagger_\downarrow(\boldsymbol{x})|0\rangle \end{aligned} \tag{2}$$

and an effective quadratic Hamiltonian, where the fermionic 2-body interaction term can be reduced to a local 2×2 effective field $\hat{V}_{\text{eff}}(\boldsymbol{x})$:

$$\begin{aligned} \hat{H}_{\text{eff}} =& \hat{H}_1 + \int d\boldsymbol{x} \left\{ \hat{\xi}^\dagger(\boldsymbol{x}) \hat{V}_{\text{eff}}(\boldsymbol{x}) \hat{\xi}(\boldsymbol{x}) \right\}, \\ \hat{H}_1 =& \int d\boldsymbol{x} \hat{\xi}^\dagger(\boldsymbol{x}) \hat{h}_1(\boldsymbol{x}, \boldsymbol{p}) \hat{\xi}(\boldsymbol{x}) \\ \hat{\xi}(\boldsymbol{x}) =& \begin{pmatrix} \hat{\xi}_\uparrow(\boldsymbol{x}) \\ \hat{\xi}_\downarrow(\boldsymbol{x}) \end{pmatrix} \quad \hat{\xi}^\dagger(\boldsymbol{x}) = \begin{pmatrix} \hat{\xi}^\dagger_\uparrow(\boldsymbol{x}) & \hat{\xi}^\dagger_\downarrow(\boldsymbol{x}) \end{pmatrix} \end{aligned} \tag{3}$$

such that the quadratic effective Hamiltonian gives exact ground state energy and the low-lying single fermion excitation energy in the thermodynamic limit. Furthermore, the self-consistent ground state $|\text{Gnd}\rangle$ solved from the effective quadratic Hamiltonian above must satisfy the following self-consistent condition

$$\hat{\xi}_\uparrow(\boldsymbol{x})\hat{\xi}_\downarrow(\boldsymbol{x})|\text{Gnd}\rangle = 0, \quad \forall \boldsymbol{x} \tag{4}$$

in addition to the usual charge-conservation condition

$$\int d\boldsymbol{x} \sum_\sigma \langle \text{Gnd}|\hat{\psi}^\dagger_\sigma(\boldsymbol{x})\hat{\psi}_\sigma(\boldsymbol{x})|\text{Gnd}\rangle = N \tag{5}$$

The total energy functional for ground state at $\{\alpha(\boldsymbol{x}), \beta(\boldsymbol{x})\}$ is thus

$$\begin{aligned} & E_{\text{Gnd}}(\{\alpha(\boldsymbol{x}), \beta(\boldsymbol{x})\}) = \langle \hat{H}_1 \rangle + \langle \text{Gnd}|\hat{H}_2|\text{Gnd}\rangle \\ & \langle \hat{H}_1 \rangle = \sum_{\varepsilon_i \le \mu} \varepsilon_i - \int d\boldsymbol{x} \left\{ \hat{\xi}^\dagger(\boldsymbol{x}) \hat{V}_{\text{eff}}(\boldsymbol{x}) \hat{\xi}(\boldsymbol{x}) \right\} \\ & \langle \hat{\xi}(\boldsymbol{x})\hat{\xi}^\dagger(\boldsymbol{x}) \rangle = \langle \text{Gnd}|\hat{\xi}(\boldsymbol{x})\hat{\xi}^\dagger(\boldsymbol{x})|\text{Gnd}\rangle \end{aligned} \tag{6}$$

where μ is the Lagrangian multiplier for the charge conservation condition, a.k.a the chemical potential or Fermi energy, and ε_i are the eigenvalues of the single particle quadratic effective Hamiltonian

$$\hat{h}_{\text{eff}}(\boldsymbol{x}, \boldsymbol{p}) = \hat{h}_1(\boldsymbol{x}, \boldsymbol{p}) + \hat{V}_{\text{eff}}(\boldsymbol{x}) \tag{7}$$

It is important to note that the self-consistent condition Eq. (4) is much more stringent than just the expectation value of the ξ-paring operator is zero. To gain some intuition on the non-double-occupancy of ξ-particles in the ground state for a quadratic effective 2×2 Hamiltonian, a discussion on the relationship of the many-body quadratic Hamiltonian to the single-particle solution to the related single-particle Hamiltonian is in order. Similar to Dirac equation for single electron, the single particle effective Hamiltonian is a 4 matrix Hamiltonian. Its eigenvalues and eigenstates are those of single particle energies and wavefunctions. The many-body ground state is a filled Fermi sea of the single particle states up to the level of total charge of the system. Thus, the variational many-body wavefunction for the ground state is

$$|\text{Gnd}\rangle = \prod_{i \in \{i|\varepsilon_i \le \mu\}} \hat{\gamma}^\dagger_i |\text{Vac}\rangle, \quad |\text{Vac}\rangle = \prod_{\boldsymbol{x}} |\text{Vac}(\boldsymbol{x})\rangle \tag{8}$$

where

$$\hat{H}_{\text{eff}} = \sum_i \varepsilon_i \hat{\gamma}^\dagger_i \hat{\gamma}_i, \quad \hat{\gamma}|Vac\rangle = 0 \tag{9}$$

and each $\hat{\gamma}_i$ corresponds to an eigenstate $\varphi_i(\boldsymbol{x})$ of the

* xdwang@sophyicstech.com

single-particle Hamiltonian

$$\hat{\gamma}_i = \int d\boldsymbol{x} \sum_\sigma \varphi_i^\dagger(\boldsymbol{x})\hat{\xi}(\boldsymbol{x}), \quad \hat{\xi}(\boldsymbol{x}) = \mathcal{U}(\boldsymbol{x}) \begin{pmatrix} \hat{\psi}_\uparrow(\boldsymbol{x}) \\ \hat{\psi}_\downarrow(\boldsymbol{x}) \\ \hat{\psi}_\downarrow^\dagger(\boldsymbol{x}) \\ \hat{\psi}_\uparrow^\dagger(\boldsymbol{x}) \end{pmatrix} \tag{10}$$

$$\hat{h}_{\text{eff}}(\boldsymbol{x},\boldsymbol{p})\mathcal{U}(\boldsymbol{x})\varphi_i(\boldsymbol{x}) = \varepsilon_i(\boldsymbol{x})\varphi_i(\boldsymbol{x}) \tag{11}$$

$$\mathcal{U}(\boldsymbol{x}) = \begin{pmatrix} -\alpha(\boldsymbol{x}) & 0 & \beta(\boldsymbol{x}) & 0 \\ 0 & \beta^*(\boldsymbol{x}) & 0 & \alpha^*(\boldsymbol{x}) \end{pmatrix} \tag{12}$$

Note that in ψ-representation, each γ annihilation operator is a mixture of ψ creation and annihilation operators. The self-consistent constraint Eq. (4) simply enforces that

$$|\text{Gnd}\rangle = \left(1 + c_\uparrow\hat{\Gamma}_\uparrow^\dagger + c_\downarrow\hat{\Gamma}_\downarrow^\dagger\right)|\text{Vac}\rangle \tag{13}$$

Note that we have truncated the 4×4 Bogolyubov transformation to 4×2 due to the ground state constraint. For excited states, since the vacuum state is not empty, we shall put back the anti-particle states to allow particle-hole pair excitations. Thus we recover the second quantized Dirac-Hamiltonian

$$\begin{aligned} \hat{H} &= \int d\boldsymbol{x}\mathcal{N}\{\hat{\Xi}^\dagger(\boldsymbol{x})\hat{h}_{Dirac}\hat{\Xi}(\boldsymbol{x})\} \\ \hat{\Xi}^\dagger(\boldsymbol{x}) &= \left(\hat{\xi}_\uparrow^\dagger(\boldsymbol{x}) \;\; \hat{\xi}_\downarrow^\dagger(\boldsymbol{x}) \;\; \hat{\xi}_\downarrow(\boldsymbol{x}) \;\; \hat{\xi}_\uparrow(\boldsymbol{x})\right) \end{aligned} \tag{14}$$

where $\mathcal{N}$ denotes the normal ordering operator, which preserves the self-consistent constraint.

Next, we will show how to construct the effective local tensor field for systems of long range 2-body interactions. The second quantized form of a general 2-body interaction in ψ-representation is

$$\begin{aligned} \hat{\mathcal{H}}_2 =& \frac{1}{2}\sum_{\sigma,\sigma';\lambda,\lambda'} \int\int d\boldsymbol{x}d\boldsymbol{x}' V(\boldsymbol{x}-\boldsymbol{x}')\mathcal{J}_{\sigma,\lambda;\sigma',\lambda'} \\ & \hat{\psi}_\sigma^\dagger(\boldsymbol{x})\hat{\psi}_{\sigma'}^\dagger(\boldsymbol{x}')\hat{\psi}_{\lambda'}(\boldsymbol{x}')\hat{\psi}_\lambda(\boldsymbol{x}) \\ =& \frac{1}{2}\sum_{\sigma,\sigma';\lambda,\lambda'} \int\int d\boldsymbol{x}d\boldsymbol{x}' V(\boldsymbol{x}-\boldsymbol{x}')\mathcal{J}_{\sigma,\lambda;\sigma',\lambda'} \\ & \hat{\psi}_\sigma^\dagger(\boldsymbol{x})\left(\hat{\psi}_\lambda(\boldsymbol{x})\hat{\psi}_{\sigma'}^\dagger(\boldsymbol{x}') - \delta(\boldsymbol{x}-\boldsymbol{x}')\delta_{\lambda,\sigma'}\right)\hat{\psi}_{\lambda'}(\boldsymbol{x}') \\ =& \hat{H}_2 + \hat{H}_U \end{aligned} \tag{15}$$

where the spatial off-diagonal interaction $\hat{H}_2$ is

$$\begin{aligned} \hat{H}_2 =& \frac{1}{2}\sum_{\sigma,\sigma';\lambda,\lambda'} \int\int d\boldsymbol{x}d\boldsymbol{x}' V(\boldsymbol{x}-\boldsymbol{x}')\mathcal{J}_{\sigma,\lambda;\sigma',\lambda'} \\ & \hat{\psi}_\sigma^\dagger(\boldsymbol{x})\hat{\psi}_\lambda(\boldsymbol{x})\hat{\psi}_{\sigma'}^\dagger(\boldsymbol{x}')\hat{\psi}_{\lambda'}(\boldsymbol{x}') \end{aligned} \tag{16}$$

and the self-interaction, a.k.a. the Hubbard term in continuum limit, is

$$\hat{H}_U = \int d\boldsymbol{x} V(0)\hat{n}_\uparrow(\boldsymbol{x})\hat{n}_\downarrow(\boldsymbol{x}), \quad \hat{n}_\sigma(\boldsymbol{x}) = \hat{\psi}_\sigma^\dagger(\boldsymbol{x})\hat{\psi}_\sigma(\boldsymbol{x}) \tag{17}$$

In simplifying the self-interaction term we have used the following property for spin-isotropic interactions such as Coulomb interaction

$$\mathcal{J}_{\sigma,\lambda;\sigma',\lambda'} = \delta_{\sigma,\lambda}\delta_{\sigma',\lambda'} - \delta_{\sigma,\lambda'}\delta_{\sigma',\lambda}\delta_{\sigma,-\lambda} \tag{18}$$

Take the square of the following identity

$$\hat{\psi}_\uparrow^\dagger(\boldsymbol{x})\hat{\psi}_\uparrow(\boldsymbol{x}) - \hat{\psi}_\downarrow^\dagger(\boldsymbol{x})\hat{\psi}_\downarrow(\boldsymbol{x}) = \hat{\xi}_\uparrow^\dagger(\boldsymbol{x})\hat{\xi}_\uparrow(\boldsymbol{x}) - \hat{\xi}_\downarrow^\dagger(\boldsymbol{x})\hat{\xi}_\downarrow(\boldsymbol{x}) \tag{19}$$

and use $\hat{n}_\sigma^2 = \hat{n}_\sigma$ we have

$$\hat{n}_\uparrow\hat{n}_\downarrow = \hat{n}_{\xi\uparrow}\hat{n}_{\xi\downarrow} + \frac{\hat{n}-\hat{n}_\xi}{2} \tag{20}$$

Thus, the self-consistent condition Eq. (4) effectively renormalizes away effect of $\hat{n}_{\xi\uparrow}\hat{n}_{\xi\downarrow}$ on ground state and single-fermion excitations, and the remaining self-interaction term $\frac{\hat{n}-\hat{n}_\xi}{2}$ can be renormalized away by a diagonal shifting of chemical potential, or zero point energy.

Thus the local effective tensor field in ψ-representation is

$$\hat{V}_{\text{eff}}(\boldsymbol{x}) = \hat{V}_0(\boldsymbol{x}) + \hat{V}_{\text{ex}}(\boldsymbol{x}) \tag{21}$$

where the diagonal-potential $\hat{V}_0(\boldsymbol{x})$ in ψ-representation is

$$\hat{V}_0(\boldsymbol{x}) = \frac{1}{2}\left(\int d\boldsymbol{x}'\rho(\boldsymbol{x}')V(\boldsymbol{x}-\boldsymbol{x}')|\right)\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{22}$$

where

$$\rho(\boldsymbol{x}) = \sum_\sigma \langle\text{Gnd}|\hat{\psi}_\sigma^\dagger(\boldsymbol{x})\hat{\psi}_\sigma(\boldsymbol{x})|\text{Gnd}\rangle \tag{23}$$

And by defining

$$V_{\lambda,\sigma}(\boldsymbol{x}) = -\frac{1}{2}\int d\boldsymbol{x}' V(\boldsymbol{x}-\boldsymbol{x}')\langle\hat{\psi}_\lambda^\dagger(\boldsymbol{x}')\hat{\psi}_\sigma(\boldsymbol{x}')\rangle \tag{24}$$

we have the local exchange potential in ψ-representation as

$$\hat{V}_{\text{ex}}(\boldsymbol{x}) = \begin{pmatrix} 0 & V_{\uparrow\downarrow}(\boldsymbol{x}) & 0 & 0 \\ V_{\downarrow\uparrow}(\boldsymbol{x}) & 0 & 0 & 0 \\ 0 & 0 & 0 & -V_{\uparrow\downarrow}(\boldsymbol{x}) \\ 0 & 0 & -V_{\downarrow\uparrow}(\boldsymbol{x}) & 0 \end{pmatrix} \tag{25}$$

Now use the Dirac Hamiltonian for our $\hat{h}(\boldsymbol{x},\boldsymbol{p})$,

$$\hat{h}(\boldsymbol{x},\boldsymbol{p}) = \hat{h}_{Dirac} = \begin{pmatrix} m_0 I_2 & \sigma\cdot\boldsymbol{p} \\ \sigma\cdot\boldsymbol{p} & -m_0 I_2 \end{pmatrix} \tag{26}$$

we have

$$\hat{h}_{\text{eff}} = \hat{h}_{Dirac} + \hat{V}_{\text{eff}} \tag{27}$$

For homogeneous system, $\hat{V}_{\text{eff}}$ is a constant matrix. The implication of a non-zero off-diagonal potential $V_{\uparrow\downarrow}(\boldsymbol{x})$ in $\hat{V}_{\text{eff}}$ is that the degeneracy of the Dirac equation is lifted and the eigenvalues of the Dirac equation at moment $\boldsymbol{k}$ becomes

$$\begin{aligned} \varepsilon_{\nu+e}(\boldsymbol{k}) &= \sqrt{(m_e + 2|V_{\uparrow\downarrow}|)^2 + \boldsymbol{k}^2} \\ \varepsilon_e(\boldsymbol{k}) &= \sqrt{m_e^2 + \boldsymbol{k}^2} \end{aligned} \tag{28}$$

where m_e is the renormalized electron mass. Assuming all electron mass comes from Coulomb interactions, we have

$$|V_{\uparrow\downarrow}|/m_e = |\rho_{\uparrow\downarrow}|/\rho = \left(|\beta|^2 - |\alpha|^2\right) / \left(2|\beta|^2\right) \tag{29}$$

To conclude, we have obtained the self-consistent ground state for any fermionic systems. The low-energy excitations of the system has two modes, one is of an effective quantized charge and the other does not. The second mode, since it is charge-less, may be identified with Majorana fermion and the other is the original electron. Note that the Majorana mode is actually the a shadow of the original fermion cast by the nonempty vacuum and is always associated with the original particle. So it is more like a resonance. Another thing to be noted is that the resonance frequency, depends on the details of the external field and the underlying off-diagonal single-fermion density matrix element, thus much less stable than the renormalized electron mass.

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[1] X. Wang, X. Chen, L. Ke, H.-P. Cheng, and B. N. Harmon, “Exact self-consistent effective hamiltonian theory,” (2020), arXiv:2010.15192 [cond-mat.str-el].