Equality of Bulk Wave Functions and Edge Correlations in Some Topological Superconductors: A Spacetime Derivation

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Equality of bulk wave functions and edge correlations in some topological superconductors: A spacetime derivation.

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For certain systems, the N-particle ground-state wavefunctions of the bulk happen to be exactly equal to the N-point space-time correlation functions at the edge, in the infrared limit. We show why this had to be so for a class of topological superconductors, beginning with the p+ip state in D=2+1. Varying the chemical potential as a function of Euclidean *time* between weak and strong pairing states is shown to extract the wavefunction. Then a Euclidean rotation that exchanges time and space and approximate Lorentz invariance lead to the edge connection. This framework readily generalizes to other dimensions. We illustrate it with a D=3+1 example, superfluid ^{3}He- B, and a p-wave superfluid in D=1+1. Our method works only when particle number is not conserved, as in superconductors.

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The boundaries or edges of condensed matter systems received scant attention until recent developments showed them to be fertile areas of research both in the Fractional Quantum Hall Effect (FQHE)[1,2]. and in topological insulators and superconductors[3–9].

In two spatial dimensions, the edge dynamics is described by conformal field theory[2] which was also used to produce wave functions in the bulk[10,11]. Moore and Read[10] showed that one may view the FQHE wavefunctions and the quasi-hole excitations as conformal blocks in which both electrons and the quasiparticle coordinates are treated on the same footing and their charges and braiding properties are severely constrained. For an exhaustive review of many related topics see Nayak *et al*[12].

We discuss problems where the N-particle ground-state wavefunctions of the bulk happen to be exactly equal to the N-point space-time correlation functions at the edge, in the infrared limit. What are the minimal ingredients necessary to establish this equality? Are analytic functions or d=2 conformal invariance required? We show that our edge-bulk equality follows for a class of topological superconductors in various dimensions invoking *only* approximate Lorentz symmetry. The connections obtained here using an effective low energy hamiltonian differ from CS theory[13] in which the hamiltonian vanishes and only non-dynamical particles enter via Wilson loops, as reviewed in Ref.12.

To relate wavefunctions, which are defined at equal time, to spacetime edge correlations, it is convenient to use the Euclidean path integral formalism, which does not single out time. A key result is a path integral representation of $Z(J)$, the generating function of N-body bulk wavefunctions. This is accomplished by introducing a time dependent chemical potential that changes abruptly at some Euclidean time. This procedure only works for particle non-conserving problems, hence the restriction to superconductors. We then drop some high derivative terms which do not matter in the infrared, and express $Z(J)$ as a Grassmann integral over a Lorentz invariant action. Rotating by 90 degrees to exchange time and a spatial direction we obtain the *same* topological superconductor but with a spatial edge induced by the jump in chemical potential. We find that the same $Z(J)$ has now morphed into the generating function for the edge correlation functions. Three examples are given: the $p+ip$ superconductor in $D=2+1$, ^{3} He B phase in $D=3+1$ and a p-wave superconductor (the Ising model) in $D=1+1$.

Extracting Wavefunctions: Recall that given a second-quantized N-body state $|\Phi\rangle$ with wavefunction $\phi(x_1,x_2,..x_N)$ we extract ϕ using

$$\phi(x_1,x_2,..x_N) = \langle\emptyset|\Psi(x_1)...\Psi(x_N)|\Phi\rangle. \tag{1}$$

where $\langle\emptyset|$ is the Fock vacuum and Ψ is the canonical electron destruction operator. For problems with variable number of particles, let us define the generating function

$$Z(J) \;=\; \langle\emptyset|e^{\int dx J(x)\Psi(x)}|\Phi\rangle \tag{2}$$

which yields N-body wavefunctions upon differentiating N- times with respect to the Grassmann source $J(x)$.

We want to express $Z(J)$ as a path integral when $|\Phi\rangle$ is the ground state of a Hamiltonian H without conserved particle number. Since Euclidean time evolution for long times projects to the ground state, we can obtain $|\Phi\rangle$ as

$$|\Phi\rangle = U(0^-,-\infty)|i\rangle \tag{3}$$

where $|i\rangle$ is a generic initial state and $U(0^-,-\infty)$ is the imaginary time propagator from $-\infty$ to 0^-. Then we insert the operator $\exp\left[\int J(x)\Psi(x)dx\right]$ at time 0. Finally, we obtain the Fock vacuum by evolving a generic state $\langle f|$ from time $+\infty$ to 0^+ using a hamiltonian H' with a huge negative μ that empties out fermions so that we may write $\langle\emptyset| = \langle f|U(\infty,0^+)$. Thus

$$Z(J) = \langle f|U(\infty,0^+)e^{\int J(x)\Psi(x)dx}U(0^-,-\infty)|i\rangle \tag{4}$$

which has a path integral representation.

Example 1: $p+ip$: The mean-field hamiltonian is[15,16]

$$H = \sum_k (c_k^\dagger, c_{-k}) \begin{pmatrix} \alpha k^2-\mu & \Delta\cdot(k_1-ik_2) \\ \Delta^*\cdot(k_1+ik_2) & -(\alpha k^2-\mu) \end{pmatrix} \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix} \tag{5}$$

where 1, 2 are spatial indices and x_3 will be time. We retain the minimum k dependence in the pairing function, and set the coefficient $\Delta = 1$ so that the gap function is $\Delta(k_1, k_2) = k_1 - ik_2$ Why then do we display the less relevant αk^2 term in the kinetic energy? The answer is that without it, the physics is insensitive to the sign of μ. But as Read and Green show, it is what allows us to associate the topologically trivial and nontrivial states with $\mu < 0$ and $\mu > 0$, with the latter containing fermions with momenta $\alpha k^2 \leq \mu$. Once we bear in mind this connection between the sign of μ and the topology, *we drop it in the subsequent computation of infrared wave functions.*

Now the mean field Hamiltonian in real space

$$H = \int d^2x \left[\Psi^\dagger(-\mu)\Psi + \frac{1}{2}(\Psi^\dagger(-i\partial_1 - \partial_2)\Psi^\dagger + h.c)\right]. \quad (6)$$

leads to corresponding Grassmann action for $U(0, -\infty)$:

$$S = \int_{-\infty}^{\infty} d^2x \int_{-\infty}^{0} dx_3 \left[\bar{\psi}\mathcal{D}\psi + \bar{\psi}i\partial\bar{\psi} + \psi i\bar{\partial}\psi\right] \quad (7)$$

$$\mathcal{D} = (-\partial_3 + \mu) \qquad \partial = \frac{\partial}{\partial z} \qquad \bar{\partial} = \frac{\partial}{\partial \bar{z}} \quad (8)$$

For the $0^+ < x_3 < \infty$, we choose $\mu = \mu_+$, a very large negative number, associated with the Fock vacuum and obtain, for all x_3, the action including the source J:

$$S(J) = \int_{-\infty}^{\infty} d^3x \left[\bar{\psi}\mathcal{D}\psi + \bar{\psi}i\partial\bar{\psi} + \psi i\bar{\partial}\psi + J\psi\delta(x_3)\right] \quad (9)$$

where $\mathcal{D}$ now contains a time-dependent $\mu(x_3)$ that jumps at $x_3 = 0$ from $\mu_- > 0$ to $\mu_+ \to -\infty$.

The generating function of the BCS wavefunctions is

$$Z(J) = \frac{\int \left[d\bar{\psi}d\psi\right] e^{S(J)}}{\int \left[d\bar{\psi}d\psi\right] e^{S(0)}} \quad (10)$$

The story is depicted in the left half of Figure 1: the fermions travel unsuspectingly along in Euclidean time x_3 and slam like bugs onto the windshield at $x_3 = 0^-$ when $\delta(x_3)J\psi$ kills them.

Since ψ and $\bar{\psi}$ in Eq. 9 are independent Grassmann variables, we integrate out $\bar{\psi}$ to obtain the effective action for just ψ to which alone J couples:

$$S_{eff}(\psi, J) = \int d^3x \left(\psi i\bar{\partial}\psi + J\psi + \psi\frac{1}{4i\partial}\mathcal{D}^T\mathcal{D}\psi\right)$$
$$\equiv S_0(J) + S_{ind}. \quad (11)$$

For the infrared limit we keep just the Jackiw-Rebbi zero mode[17] of the hermitian operator

$$\mathcal{D}^T\mathcal{D}(x_3) = (\partial_3 + \mu(x_3))(-\partial_3 + \mu(x_3)), \quad (12)$$

that obeys $\mathcal{D}f_0 = 0$

$$f_0(x_3) = f_0(0)e^{\int_0^{x_3}\mu(x')dx'} \quad (13)$$

in the mode expansion of the Grassmann field:

$$\psi(x_1, x_2, x_3) = f_0(x_3)\psi(x_1, x_2). \quad (14)$$

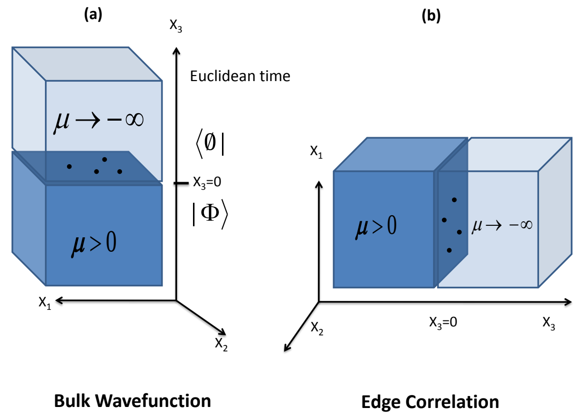

FIG. 1: (a) Wavefunction: The original superconductor with $\mu = \mu_- > 0$ lies in the $x_1 - x_2$ plane and evolves in Euclidean time x_3 from $-\infty$ to 0^-, projecting out the ground state $|\Phi\rangle$. At $x_3 = 0^+$ the chemical potential drops abruptly to a large negative value μ^-, leading to the Fock vacuum. (b) Correlation functions: A Lorentz rotation makes x_1 the new time and x_3 a the spatial coordinate along which the system has an edge at $x_3 = 0$. The world-sheet of the edge lies in the $x_1 - x_2$ plane at $x_3 = 0$.

This kills S_{ind}, and upon integrating f_0^2 over x_3,

$$S_{eff}(J) = \int dx_1 dx_2\, \psi(i\bar{\partial} + Jf_0(0))\psi \quad (15)$$

While this is indeed the action of a chiral majorana fermion living in the $1-2$ plane we are not done: we need to show that this fermion and this action also arise at the edge of the *same* $p + ip$ system. But so far we have no edge! It will be introduced shortly, but first a summary of results on the wavefunction.

Pfaffian Wavefunction: Integrating over ψ in Eq. 15, and suppressing the constant $f_0^2(0)$) we find

$$Z(J) = \exp\left[\int d^2\mathbf{r}J(\mathbf{r})\left[\frac{1}{4i\bar{\partial}}\right]_{\mathbf{rr}'} J(\mathbf{r}')\right] \quad (16)$$

The two-particle wavefunction $\phi(\mathbf{r}_1 - \mathbf{r}_2)$ can be written in terms of many related quantities:

$$\phi = \frac{\partial^2 Z(J)}{\partial J_1 \partial J_2} = \left[\frac{1}{2i\bar{\partial}}\right]_{\mathbf{r}_1\mathbf{r}_2} = \Delta^{*-1}_{\mathbf{r}_1\mathbf{r}_2} = \frac{1}{z_1 - z_2} \quad (17)$$

and the N-particle wavefunction is $\mathrm{Pf}(\frac{1}{z_i - z_j})$. In 18 we relate $Z(J)$ and the conventional BCS wavefunction:

$$|BCS\rangle = \exp\left(\frac{1}{2}\int \Psi^\dagger(x)g(x-y)\Psi^\dagger(y)dxdy\right)|\emptyset\rangle \quad (18)$$

and see that $\phi = -g(\mathbf{r}_1 - \mathbf{r}_2)$.

The Edge: To relate $Z(J)$ in Eqn. 9 to a problem with the edge we rewrite $S(J)$ in Lorentz invariant form:

$$S(J) = \int d^3x \left[\bar{\Psi}\left(\partial\!\!\!/ - \mu\right)\Psi + J^T\Psi\right] \quad \text{where} \tag{19}$$

$$\Psi = \begin{pmatrix} \psi \\ \bar{\psi} \end{pmatrix} \quad \bar{\Psi} = \Psi^T\varepsilon; \quad \varepsilon = i\sigma_2 \quad \partial\!\!\!/ = \gamma_\mu\partial_\mu \tag{20}$$

$$\gamma_1 = \sigma_2 \quad \gamma_2 = -\sigma_1 \quad \gamma_3 = \sigma_3 \tag{21}$$

$$J^T = J\delta(x_3)(1\,0). \tag{22}$$

Look at the left half of Figure 1. We see our current description of the superconductor: translationally invariant in the $x_1 - x_2$ plane, regarded as the space in which the p_1+ip_2 superconductor lives, and with a jump in μ at "time" $x_3 = 0$. In this description, the functional integral is saturated by one mode $f_0(x_3)$, glued to the interface, exactly like the electron gas at a heterojunction.

Extracting $H(x_1, x_2)$ from the Lorentz invariant action is like taking the row-to row transfer matrix. To derive the hamiltonian that governs the column-to -column dynamics, we rotate the three dimensional spacetime by $-\frac{\pi}{2}$ around the x_2 axis to obtain the view shown in the right half of Figure 1. The points carry the same labels as before but the spinor undergoes a rotation:

$$\Psi = \begin{pmatrix} \psi \\ \bar{\psi} \end{pmatrix} = e^{i\frac{\pi}{4}i\gamma_3\gamma_1}\begin{pmatrix} \psi' \\ \bar{\psi}' \end{pmatrix} = e^{i\frac{\pi}{4}\sigma_1}\Psi' \tag{23}$$

Upon performing this transformation we end up with

$$S(\Psi', J) = \int d^3x \left[\bar{\Psi}'\left[\sigma_3\partial_1 - \sigma_1\partial_2 - \sigma_2\partial_3 - \mu\right]\Psi' + J\delta(x_3)\left(\frac{\psi' + i\bar{\psi}'}{\sqrt{2}}\right)\right] \tag{24}$$

which describes exactly the same $p + ip$ superconductor but in the $2-3$ plane (with $1 \to 3, 3 \to -1$) with an edge at $x_3 = 0$ with the $\mu > 0$ side containing the nontrivial superconductor.

To see that the field $\frac{\psi' + i\bar{\psi}'}{\sqrt{2}}$ that J couples to is precisely the Majorana field that arises at the edge, consider solving the equation for the zero mode which follows from Eq. 24 on dropping all x_1, x_2 dependence:

$$(\sigma_2\partial_3 + \mu(x_3))\chi_0' = 0 \Rightarrow \chi_0'(x_3) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} f_0(x_3). \tag{25}$$

the normalizable spinor solution indeed corresponds to the operator $\frac{1}{\sqrt{2}}(\psi' + i\psi'^\dagger)$.

We are done, for we have shown that $Z(J)$ is at once the generators of electronic wavefunction in the bulk and of correlation functions of the Majorana field at the edge.

For completeness, the edge Majorana field action follows from saturating the x_3 dependence of Ψ' as follows:

$$\Psi'(x_1, x_2, x_3) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} f_0(x_3)\psi'(x_1, x_2) \tag{26}$$

Plugging this into the action $S(\Psi', J)$ one finds, upon integrating the normalized function $f_0'(x_3)$ over x_3

$$S(\Psi', J) \to \int dx_1 dx_2 \left[\psi' i\bar{\partial}\psi' + Jf_0(0)\psi'\right] \tag{27}$$

exactly as in Eqn.15, for the wavefunction.

Example 2: $^3He - B$ in D=3+1: In a simplified model of superfluid $^3He - B$, Cooper pairs have spin 1, whose projection lies perpendicular to the momenta $\pm\mathbf{k}$[20,21]. The winding of this axis around the Fermi surface in the weak pairing phase leads to its topological properties[21,22]. The mean-field Hamiltonian for this time-reversal invariant class DIII system is[20,21] is:

$$H = \sum_{\mathbf{p}\sigma\sigma'} \Psi^\dagger_{\mathbf{p}\sigma}\left(\frac{\mathbf{k}^2}{2m} - \mu\right)\Psi_{\mathbf{k}\sigma} + \{\Delta_{\mathbf{k}\sigma\sigma'}\psi_{\mathbf{k}\sigma}\psi_{-\mathbf{k}\sigma'} + \text{h.c.}\} \tag{28}$$

$$\Delta_{\mathbf{k}\sigma\sigma'} = [\varepsilon\mathbf{k}\cdot\boldsymbol{\sigma}]_{\sigma\sigma'}$$

The $d = 3$ problem is just the $d = 2$ problem on steroids: Δ goes from being a complex number to a quaternion, and the spinless fermion is replaced by a two-component spinor. Hence the weak-pairing wavefunction is

$$g_{\sigma_i\sigma_j}(\mathbf{r}_{ij}) \sim \frac{[\mathbf{r}_{ij}\cdot\boldsymbol{\sigma}\varepsilon]_{\sigma_i\sigma_j}}{r_{ij}^3} \tag{29}$$

and the many-body wavefunction is Pf(g), as in Ref. 8:

$$\Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \ldots, \mathbf{r}_{2N}\sigma_{2N}) = \text{Pf}\left\{g_{\sigma_i\sigma_j}(\mathbf{r}_i - \mathbf{r}_j)\right\} \tag{30}$$

The Lorentz invariant action for the wavefunction is

$$S = \int d^4x \frac{1}{2}\bar{\Psi}\left[\partial\!\!\!/ - \mu\right]\Psi \quad \text{where} \tag{31}$$

$$\gamma_0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \quad \boldsymbol{\gamma} = \begin{pmatrix} 0 & i\boldsymbol{\sigma}\varepsilon \\ i\varepsilon\boldsymbol{\sigma} & 0 \end{pmatrix} \tag{32}$$

$$\bar{\Psi} = \Psi^T\begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \tag{33}$$

Now the 0 and 1 directions are exchanged by $R = \exp\left[\frac{i\pi}{2}\frac{i\gamma_0\gamma_1}{2}\right]$, so that J now couples to $\frac{\psi' + i\sigma_3\psi'^\dagger}{\sqrt{2}}$ which is readily verified, as before, to be the gapless edge mode of the rotated theory. The action for the edge theory obtained by saturating with the zero mode is

$$S_{edge} = \int d^3x \frac{1}{2}\bar{\psi}\partial\!\!\!/\psi \qquad \partial\!\!\!/ = \sigma_j\partial_j \qquad \bar{\psi} = \psi^T(-\sigma_2) \tag{34}$$

Example 3: We could equally well go *down* a dimension, to a spinless p-wave superconductor in $d = 1 + 1$[14] where $\Delta = k_x$, which is also related to the quantum Ising model, via the Jordan-Wigner mapping. The edge theory is $0 + 1$ dimensional, corresponding to a Majorana zero mode, with $\mathcal{L} = \frac{1}{2}\psi\partial_x\psi$. The pair wavefunction in the weak pairing phase is $g(x) \sim \text{Sign}(x)$.

One can use the parton construction[23,24] to generate fractionalized analogs of the free fermion phases discussed here. One such attempt, the fractionalized topological superconductor, is discussed in 18

Summary: We have explained why the electronic wavefunctions in the bulk coincided with the massless Majorana correlation functions at the edge in certain problems. We first wrote $Z(J) = \langle\emptyset|e^{J\Psi}|BCS\rangle$ as a path integral in which the chemical potential abruptly jumped at in Euclidean time. Dropping the 'k^2' terms, but not the connection they provide between the sign of μ and topology, we obtained a Lorentz invariant action. Upon rotation by $\pi/2$ the same action described a system that had an edge and $Z(J)$ had meanwhile morphed into the generating function for edge correlations.

While our trick of rotating the axes can be tried in any Euclidean path integral, Lorentz invariance is needed to ensure that the bulk for which the wavefunction is written is the same as the one with the edge after rotation. For Laughlin states realized by applying a magnetic field to fermions with a parabolic dispersion, we run into two kinds of problems: the action is far from Lorentz invariant and we cannot vary μ to drain the sea of particles since their number is conserved. We are working on deriving the appropriate bulk-boundary connection.

The bulk-boundary correspondence presented here is not limited to $D = 2+1$ and is based on the approximate Lorentz invariance of the mean-field action. It is very different from that of topological Chern-Simons theories with vanishing hamiltonian and restricted to $D = 2+1$.

Various topological superconductors are known corresponding to different Altland-Zirnbauer classes[8] - can our method be applied to *any* of them? In order to drain the Fermi sea in our derivation, the band structure should itself be trivial, and all the topology must be contained in the pairing (such as the phase winding around the Fermi surface in $p+ip$). Such a construction is possible for topological phases in class D in d=1 and d=2 (like p+ip), in class C in d=2 (like d+id) and class DIII in d=2,3 (He-3 B phase). However, it appears to be not possible for class CI in d=3,[27] which additionally rely on non-trivial topology of the weak pairing Fermi surface.

The entanglement spectrum of the bulk seems to determine the edge theory[25,26], which we now relate back to the bulk wavefunction. Since the entanglement of a gapped phase appears from near the cut, the *entire* bulk wavefunction must be coded holographically in every $d-1$ dimensional sliver probed in the entanglement analysis.

Previously, the connection between edge states and bulk wavefunctions has played an important role identifying new FQH states[10,28]. Our work suggests a similar approach could be fruitful in identifying interacting topological phases in D=3+1.

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