Translation-invariant topological superconductors on a lattice

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Translation-invariant topological superconductors on a lattice

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In this paper we introduce four $Z_2$ topological indices $\xi_k=0,1$ at $k=(0,0), (0,\pi), (\pi,0), \text{and} (\pi,\pi)$ characterizing 16 universal classes of two-dimensional superconducting states that have translation symmetry but may break any other symmetries. The 16 classes of superconducting states are distinguished by their even/odd numbers of fermions on even-by-even, even-by-odd, odd-by-even, and odd-by-odd lattices. As a result, the 16 classes topological superconducting states exist even for interacting systems. For noninteracting systems, we find that $\xi_k$ is the number of electrons on $k=(0,0)$, $k=(0,\pi)$, $k=(\pi,0)$, or $k=(\pi,\pi)$ orbitals (mod 2) in the ground state. For three-dimensional superconducting states with only translation symmetry, topological indices give rise to 256 different types of topological superconductors.

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I. INTRODUCTION

In last 20 years, it became more and more clear that Landau symmetry breaking theory1–3 cannot describe all possible orders in quantum states of matter (the states of matter at zero temperature). The new order is called topological order for gapped states. Fractional quantum-Hall systems5 and many other systems were shown to have topologically ordered ground states.6–16

Topological order can exist even if we break all symmetries. However, for systems with certain symmetries, a new type of order, symmetry protected topological order, can appear.17,18 Even though the ground states with symmetry protected topological order do not break any symmetries, they can still represent different phases of matter. The simplest example of symmetry protected topological orders is the $Z_2$ topological insulator that can appear in two-dimensional (2D) and three-dimensional (3D) free fermion systems with time-reversal symmetry.19–24 The Haldane phase in one-dimensional spin-1 chain is the oldest example of symmetry protected topological phase with time reversal, parity, and translation symmetries.18,25,26 Symmetry-protected topological order appear quite commonly in topological phases with symmetries. The projective symmetry group is introduced to (partially) characterize/distinguish different symmetry protected topological orders.17

In this paper, we study 2D fully gapped superconducting (SC) states on a lattice that have only translation symmetry. The time-reversal, spin-rotation, lattice $180^\circ$ rotation and parity, etc., may not be the symmetries of the SC Hamiltonian. The time-reversal violating SC states can be characterized by a winding number.27,28 We found that the 2D SC states with a given winding number can be further divided into eight classes. Although all those classes of SC states have the same symmetry, they cannot change into each other without quantum phase transitions which close the energy gap. So the different classes of SC states belong to different quantum phases are called topological superconductors. Our results can be easily generalized to 3D lattice which leads to 256 different topological superconductors with translation symmetry.

If we consider different symmetries (other than the translation symmetry), then different classes of topological superconductors can be obtained. In particular, the time-reversal invariant topological superconductors are studied in Refs. 29–31. The nontranslation-invariant topological superconductors with different symmetry classes are studied in Refs. 32 and 33.

In 2D, four $Z_2$ topological indices $\xi_k$ at $k=(0,0), (0,\pi), (\pi,0), \text{and} (\pi,\pi)$ are introduced to characterize 16 classes of topological SC states. The 16 classes of SC states are distinguished by their even/odd number of fermions on even-by-even (ee), even-by-odd (eo), odd-by-even (oe), and odd-by-odd (oo) lattices. We stress that the topological SC states discussed here exist even for interacting systems. Also, the topological indices $\xi_k$ can distinguish different symmetry protected topological orders that cannot be distinguished by projective symmetry group.

The paper is organized as follows. In Sec. II, we introduce the Hamiltonian of fully gapped 2D SC states with only translation symmetry. In Sec. III, we classify topological superconductors by $Z_2$ topological invariants. In Sec. IV, the physical quantum numbers separating topological SC states are studied. In Sec. V, we discuss examples of translation-invariant topological SC phases. In Sec. VI, we classify the spin-1/2 SC states with spin-orbital coupling. Finally, the conclusions are given in Sec. VII.

II. FULLY GAPPED 2D SC STATES WITH ONLY TRANSLATION SYMMETRY

We use $i=(i_x, i_y)$ to label unit cells of a lattice and $\alpha=1, 2, \ldots$ to label the electron operators $\psi_{\alpha, i}$ in the unit cell $i$. The index $\alpha$ labels the spin and/or orbitals of electrons. The 16 classes of topological SC states can already exist when $\alpha=1$ (i.e., only one electronic state per unit cell). So without losing generality, we will assume $\alpha=1$ here and drop the $\alpha$ index. In this case, the most general SC state with only translation symmetry can be described by
\[ H = \sum_{ij} \psi_i^\dagger u_{ij} \psi_j + \sum_{i} (\psi_i^\dagger \eta_i \psi_i^\dagger + \text{H.c.}), \]  
\[ (1) \]

where \( u_{ij} \) and \( \eta_i \) are complex numbers. The translation invariance requires that \( u_{ij} = u_{i+j, j+k} \) and \( \eta_i = \eta_{i+j} \). In this paper, the chemical potential is set to be zero.

One can rewrite the SC Hamiltonian in momentum space by introducing \( \Psi_k = (\psi_k) \) and \( \Psi_k^\dagger = (\psi_k^\dagger) \). Note that \( \Psi_k \) satisfy the following algebra:

\[ \{\Psi_{k'}, \Psi_k\} = \delta_{ij} \delta_{k', k}, \quad \{\Psi_{k'}, \Psi_{k'}\} = (\sigma_i)_{ij} \delta_{k, k'}, \]  
\[ (2) \]

where \( \sigma_i, i = 1, 2, 3 \) are Pauli matrices. We also note that \( (\Psi_{k'}^\dagger \Psi_{-k}) \) can be expressed in term of \( (\Psi_k^\dagger \Psi_k) \),

\[ \Psi_{-k} = \sigma_i \Psi_k^\dagger, \quad \Psi_{-k}^\dagger = \Psi_k^\dagger \sigma_i. \]  
\[ (3) \]

In terms of \( \Psi_k, H \) can be written as

\[ H = \sum_{k>0} \Psi_k^\dagger M(k) \Psi_k + \sum_{k>0} \Psi_k^\dagger M(k) \Psi_k, \]  
\[ (4) \]

where \(-\pi < k_x, k_y < \pi \) and \( M(k) = 2 \times 2 \) Hermitian matrices \( M(k) = M^\dagger(k) \). Here \( k = 0 \) means \((k_x, k_y) = (0, 0)\), \((0, \pi)\), \((\pi, 0)\), or \((\pi, \pi)\). Also \( k_x \) and \( k_y \) are quantized: \( k_x = \frac{2\pi}{L_x} \) \text{integer} and \( k_y = \frac{2\pi}{L_y} \) \text{integer}, where \( L_x \) and \( L_y \) are size of the square lattice in the \( x \) and \( y \) directions. In paper, we assume the periodic boundary condition.

Note that on an even by even lattice (i.e., \( L_x = \text{even} \) and \( L_y = \text{even} \)), \((k_x, k_y) = (0, 0)\), \((0, \pi)\), \((\pi, 0)\), or \((\pi, \pi)\) all satisfy the quantization conditions \( k_x = \frac{2\pi}{L_x} \) \text{integer} and \( k_y = \frac{2\pi}{L_y} \) \text{integer}. In this case, \( \Sigma_{k>0} \) sums over all four points \((k_x, k_y) = (0, 0)\), \((0, \pi)\), \((\pi, 0)\), and \((\pi, \pi)\). On other lattices, \( \Sigma_{k>0} \) sums over less points. Say on an odd by odd lattice, only \((k_x, k_y) = (0, 0)\) satisfies the quantization conditions \( k_x = \frac{2\pi}{L_x} \) \text{integer} and \( k_y = \frac{2\pi}{L_y} \) \text{integer}. In this case, \( \Sigma_{k>0} \) sums over only \((k_x, k_y) = (0, 0)\) point.

We note that \( \Psi^\dagger_k \Psi_k = 2. \) Thus up to a constant in \( H \), we may assume \( M(k) \) satisfy \( \text{Tr} M(k) = 0 \). Due to Eq. (3),

\[ \Psi^\dagger_k M(-k) \Psi_{-k} = \text{Tr} M(k) - \Psi^\dagger_k \sigma_i M^\dagger(-k) \sigma_i \Psi_k. \]  

Thus, we may rewrite Eq. (4) as

\[ H = \sum_{k>0} \Psi_k^\dagger U(k) \Psi_k + \frac{1}{2} \sum_{k>0} \Psi_k^\dagger U(k) \Psi_k. \]  
\[ (5) \]

\[ U(k) = M(k) - \sigma_i M^\dagger(-k) \sigma_i. \]  
\[ (6) \]

Here \( k > 0 \) means that \( k \neq 0 \) and \( k_x > 0 \) or \( k_y > 0 \). Clearly \( U(k) \) satisfies

\[ U(k) = -\sigma_i U^\dagger(-k) \sigma_i, \quad U(k) = U^\dagger(k). \]  
\[ (6) \]

Now we expand the traceless \( U(k) \) by three Pauli matrices \( \sigma_i \). We have \( U(k) = \sum_{i,j} c_i(k) \sigma_i \sigma_j \), where \( c_i(k) \) are real. From Eq. (6), we find

\[ c_i(k) = c_i(-k), \quad c_i^\dagger(k) = -c_i^\dagger(-k), \quad i = 1, 2. \]  
\[ (7) \]

Thus for odd matrices, \( c_i(k) \) are zero at momentum \((0, 0)\), \((0, \pi)\), \((\pi, 0)\), and \((\pi, \pi)\). \[ (7) \]

### III. CLASSIFICATION OF TOPOLOGICAL SUPERCONDUCTORS

For a generic choice of \( u_{ij} \) and \( \eta_i \), the corresponding SC Hamiltonian (5) is gapped. Note that the energy levels of the SC Hamiltonian (5) appear in \((E, -E)\) pairs. The SC ground state is obtained by filling all the negative energy levels. The SC Hamiltonian is gapped if the minimal positive energy is finite.

As we change the SC ansatz \( u_{ij} \) and \( \eta_i \), the SC energy gap may close which indicate a quantum phase transition. Thus if two gapped regions are always separated by a gapless region, then the two gapped regions will correspond to two different phases. We may say that the two phases carry different topological orders.

In the following, we introduce topological indices that can be calculated for each gapped SC ansatz \( (u_{ij}, \eta_i) \). We will show that two gapped SC ansatz with different topological indices cannot smoothly deform into each other without closing the energy gap. Therefore, the topological indices characterize different SC states translation symmetry.

The SC Hamiltonian in momentum space, Eq. (5), has a form as

\[ H = H(k > 0) + H(k = 0). \]  
\[ (8) \]

First, let us diagonalizing the SC Hamiltonian at the points \( k > 0 \). Introducing

\[ W(k) \Psi_k = \begin{pmatrix} \alpha_k \\ \alpha_k^\dagger \end{pmatrix}, \]  
\[ (9) \]

\[ W(k) U(k) W^\dagger(k) = \begin{pmatrix} \epsilon(k) & 0 \\ 0 & -\epsilon(k) \end{pmatrix}, \quad \epsilon(k) > 0, \]  
\[ (10) \]

we find

\[ H(k > 0) = \sum_{k > 0} \epsilon(k) (\alpha_k^\dagger \alpha_k - \alpha_{-k}^\dagger \alpha_{-k}). \]  

We note that \( \alpha_{\pm k} \) will annihilate the SC ground state, \( \alpha_{\pm k} | \Psi_{\text{SC}} \rangle = 0 \). At the four \( k = 0 \) points, the Hamiltonian is already diagonal since \( c_{1,3}(k) = 0 \).

The energy spectrum at \( k = 0 \) motivates us to introduce four \( \zeta \) as the topological indices, one for each \( k = 0 \) point,

\[ \zeta_k = 1 - \Theta[c_1(k)]. \]  
\[ (11) \]

where \( \Theta(x) = 1 \) if \( x > 0 \) and \( \Theta(x) = 0 \) if \( x < 0 \). If two SC states have different sets of topological indices \( \zeta_k = 0, \pi \), then as we deform one state smoothly into the other, some \( \zeta_k \) must change sign. When \( \zeta_{\pm k} \) change sign, then \( c_1(k) = 0 \) and the SC state becomes gapless indicating a quantum phase transition. Therefore, there are 16 different translation-invariant SC labeled by \( \zeta_k = 0, \pi \), \( \zeta_{\pm k} = 1111, 1100, 1010, 1001, 0101, 0111, 0110, 0000, 1000, 0100, 0010, 0001, 1110, 1101, 1011, \) and 0111.
IV. PHYSICAL QUANTUM NUMBERS SEPARATING TOPOLOGICAL SC STATES

In the above, we introduced 16 classes of translation-invariant SC states through the four topological indices $\zeta_{k=0}$. However, as we deform one class of SC state to another, we have assumed the range of spin/orbital index $\alpha$ to be $\alpha = 1$. If the range of $\alpha$ is more than 1, do we still have to encounter gapless region as we deform one class of SC state to another? Also, if electrons are interacting, whether different classes of SC states are still separated by gapless region?

A. Even/odd number of electrons

In this part, we show that even with many spin/orbital states per unit cell and even in the presence of weak interactions, there are still 16 classes of translation-invariant SC states. We obtain this result by finding universal physical quantum numbers that separate the 16 classes of SC states. The universal physical quantum numbers are $(-)^{N_e}$ on ee, oe, eo, and oo lattices. Here $N_{e}$ is the number of electrons in the SC ground state. Note that $(-)^{N_e}$ commutes with the SC Hamiltonian. Although $N_{e}$ is not definite in the SC ground state, $(-)^{N_e}$ is uniquely defined.

We note that $N_{e} = N_{k=0} + N_{k=0}$, where $N_{k=0} = \sum_{k\neq 0} \phi_{k}^{k} \phi_{k}^{k}$ and $N_{k=0} = \sum_{k=0} \phi_{k}^{k} \phi_{k}^{k}$. For $k > 0$, we have

$$(-)^{ \phi_{k}^{k} \phi_{k}^{k} \phi_{k}^{k} \phi_{k}^{k} - \phi_{k}^{k} \phi_{k}^{k} \phi_{k}^{k} \phi_{k}^{k} } = (-)^{ \phi_{k}^{k} \phi_{k}^{k} \phi_{k}^{k} \phi_{k}^{k} }$$

Hence we have

$$(-)^{ \phi_{k}^{k} \phi_{k}^{k} \phi_{k}^{k} \phi_{k}^{k} - \phi_{k}^{k} \phi_{k}^{k} \phi_{k}^{k} } = (-)^{ \phi_{k}^{k} \phi_{k}^{k} \phi_{k}^{k} \phi_{k}^{k} }$$

for $k > 0$. The total number of the electrons on all the $k > 0$ orbitals is always even.

So to determine if the SC ground state contain even or odd number of electrons, we only need to count the number of the electrons at the $k = 0$ points. At $k = 0$, we have

$$\phi_{k}^{k} \phi_{k}^{k} |\Psi_{SC} \rangle = (1 - \Theta(\zeta_{k}(k)) |\Psi_{SC} \rangle = \zeta_{k} |\Psi_{SC} \rangle.$$  

We see that for noninteracting electrons, the topological indices $\zeta_{k}$ at the $k = 0$ points are just the numbers of electrons in the SC ground state on the corresponding $k$ orbitals mod 2. This can be used as a definition of topological indices. If the gapped SC phase has a weak SC order, then $\zeta_{k}$ are just the numbers of electrons in the normal state on the corresponding $k$ orbitals mod 2. From the above discussion, we see that spin-singlet SC states always have $\{\zeta_{k}\} = 0000$ topological SC order.

From Eq. (14), we find that the total fermion number at the $k = 0$ points and the total number of electrons are given by

$$N_{k=0} \mod 2 = N_{e} \mod 2 = \sum_{k=0} \zeta_{k} \mod 2.$$  

Let us use the topological SC state (0100) as an example to demonstrate a detailed calculation of the total fermion number at the $k = 0$ points. Note that on even-by-even lattice, all the four $k = 0$ points $k = (0, 0), (0, \pi), (\pi, 0), (\pi, \pi)$ are allowed. In this case $\zeta_{k}$ mod 2 is the sum of all four $\zeta_{k} \equiv \zeta_{k} \mod 2$. Among the four $k = 0$ points, only $k = (0, \pi)$ point has $\zeta_{k} = 1$ as indicated by the second 1 in the label (0100). As a result, the total fermion number at the $k = 0$ points is 1 which is an odd number. We denote the case by “$-$.” On an even-by-odd lattice, only two $k = 0$ points $k = (0, 0)$ and $(\pi, \pi)$ are allowed. In this case due to $\zeta_{k} \equiv \zeta_{k} \mod 2$, the result is the same as that on an even-by-odd lattice, that is $-$. On an odd-by-odd lattice, there is only one $k = 0$ point: $k = (0, 0)$. In this case due to $\zeta_{k} \equiv \zeta_{k} \mod 2$, the result is the same to that on an even-by-odd lattice, that is $+$.

This way, Eq. (15) allows us to construct the follow table:

$$
\begin{array}{cccc}
(-)^{N_{e}} & (ee) & (eo) & (oo) \\
0000: & + & + & + \\
1111: & + & + & - \\
0101: & + & + & + \\
1010: & + & + & - \\
0011: & + & + & + \\
1100: & + & + & + \\
0110: & + & + & + \\
1011: & + & + & + \\
0100: & + & + & + \\
\end{array}
$$

We see that all 16 classes of SC states have distinct even/odd number of electrons on the four types of lattices. Since $N_{e}$ mod 2 is discrete, so it is a universal quantum number in a gapped phase that is robust against perturbations of weak mixing with other spin/orbital states and adding weak interactions. Therefore, the 16 topological SC phases is robust against weak spin/orbital mixing and weak interactions. In addition we point out that these results may reduce to those in Ref. 28 by Read and Green by considering only the point $k = (0, 0)$.

B. Edge states

In this part, we study the edge states by calculate the different classes of SC states with opening boundary condi-
tion along $x$ or $y$ direction. We find that the edge states of different classes of SC states have different structures which allow us to experimentally detect the different classes of SC states.

For the $(1000, 0100, 0010, 0001, 1110, 1101, 1011, 0111)$-type SC states we find that there exist chiral edge states. Edge spectrum crosses zero at momentum $K_x$ on edge along $x$ direction and at momentum $K_y$ on edge along $y$ direction.

For example, Figs. 1 and 2 show the edge state of topological SC state $0100$: the nodal points are fixed at $K_x=0$ on an edge along $x$ direction and $K_y=\pi$ on an edge along $y$ direction, respectively. The nodal points $(K_x, K_y)$’s for the SC states $1110, 1101, 1010, 0111$ are given in the following table:

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<th>$K_x$</th>
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For other types of SC states $1111, 1100, 0110, 0011, 1001, 0101, 1010, 0000$ with zero winding number $w$ (see detailed definition below), there may also exist gapless edge states protected by translation symmetry, which are stable against arbitrary translation-invariant perturbations. For example, Figs. 3 and 4 show the edge state of topological SC state $0110$: the nodal points are fixed at $K_x=0$ and $K_y=\pi$ on an edge along both $x$ direction and $y$ direction, respectively. The nodal points $(K_x, K_y)$’s for the SC states $1111, 1100, 0110, 0011, 1001, 0101, 1010, 0000$ are given in the following table:

<table>
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<th>$K_x$</th>
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V. EXAMPLES OF TRANSLATION-INVARIANT TOPOLOGICAL SC PHASES

Let us first consider the following $p_x+ip_y$ SC state:

\[
H = \sum_{ij} \left( \phi_i^\dagger u_{ij} \phi_j + \psi_i \eta_{ij} \psi_j + \text{H.c.} \right),
\]

\[
u_{i,\pm x} = u_{i,\pm y} = -\chi_1, \quad u_{i,\pm x+y} = u_{i,\mp x-y} = -\chi_2.
\]

\[
\eta_{i,\pm x} = \eta, \quad \eta_{i,\pm y} = i \eta.
\]

We find that

\[
c_3(k) = -2\chi_1[\cos(k_x) + \cos(k_y)] - 2\chi_2[\cos(k_x + k_y) + \cos(k_x - k_y)].
\]
\[ c_i(k) = 2\eta \sin(k_i), \quad c_i(k) = 2\eta \sin(k_i). \]  
Assume \( \chi_1 > 0 \), we find that when \( \chi_2 > 0 \) the SC state is a \( \{ \xi_4 \} = 1000 \) topological superconductor. When \( -\chi_1 < \chi_2 < 0 \), the SC state is a \( \{ \xi_5 \} = 1110 \) topological superconductor. When \( \chi_2 < -\chi_1 \), the SC state is a \( \{ \xi_6 \} = 0110 \) topological superconductor.

The \( p_x + ip_y \) topological superconductor is also characterized by a winding number \( w \) which is given by \( w = \text{sgn}(\eta) \) for the \( \chi_2 > 0 \) case.\(^{28}\) We like to point out that in general the winding number satisfies

\[ w \mod 2 = \xi(0,0) + \xi(\pi,0) + \xi(0,\pi) + \xi(\pi,\pi) \mod 2. \]

The above result implies that the topological indices \( \{ \xi_k \} \) do not provide a complete characterization of topological order, i.e., for a given set of \( \{ \xi_k \} \), there can still be different topological phases distinguished by some other topological quantum numbers, such as the winding number.

**VI. SPIN-1/2 SC STATES WITH SPIN-ORBITAL COUPLING**

Let us consider spin-1/2 SC states with spin-orbital coupling in more detail. We need to consider a more general case where there are two spin/orbital states per unit cell. In this case, the most general SC state with only translation symmetry is described by

\[ H = \sum_{\eta} \psi_0^\dagger u_{\eta} \psi_{\eta} + \sum_{\eta} (\psi_{\eta}^\dagger \eta_{\eta} \psi_{\eta}^\dagger + \text{H.c.}), \]

where \( u_{\eta} \) and \( \eta_{\eta} \) are \( 2 \times 2 \) matrices. One can rewrite the SC Hamiltonian in momentum space by introducing \( \Psi_k = (\psi_{1,k}, \psi_{1,-k}, \psi_{2,k}, \psi_{2,-k}) \).

\[ H = \sum_{k > 0} \Psi_k^\dagger U(k) \Psi_k + \frac{1}{2} \sum_{k > 0} \Psi_k^\dagger U(k) \Psi_k, \]

where \( U(k) \) satisfies \( U(k) = -\Gamma U^T(-k) \Gamma \), \( U(k) = U^l(k), \) and \( \Gamma = \sigma_1 \otimes \sigma_0 \). We can expand \( U(k) \) by 16 Hermitian matrices \( M_{(a\beta)} = \sigma_a \otimes \sigma_\beta \), \( \alpha, \beta = 0,1,2,3 \), where \( \sigma_0 = 1 \). We have

\[ U(k) = \sum_{(a\beta)} c_{(a\beta)}(k) M_{(a\beta)}, \]

where \( c_{(a\beta)}(k) \) are real. We find that at the four \( k = 0 \) points, only \( c_{(30)}, c_{(12)}, c_{(22)}, c_{(33)}, c_{(31)} \), and \( c_{(02)} \) are nonzero. The topological indices at \( k = 0 \) points are

\[ \xi_k = 1 - \Theta[c_{(30)}(k) + c_{(12)}^2(k) + c_{(22)}^2(k) - c_{(33)}^2(k)] \]

This equation allows us to calculate \( \xi_k \) for spin-1/2 superconductors that may break spin-rotation symmetry.

**VII. CONCLUSION**

Using the even/odd numbers of electrons at the four \( k = 0 \) orbitals, we find that a gapped 2D SC states with translation symmetry can be in one of 16 topological SC phases. Those 16 classes of SC phases have different even/odd numbers of electrons on even-by-even, even-by-odd, odd-by-even, and odd-by-odd lattices. This result can be easily generalized to any dimensions. We find that there are 256 \((2^{24})\) different topological SC orders in three dimensions \((d \text{ dimensions})\). Such topological SC orders are robust against weak interactions that do not break the translation symmetry.

**ACKNOWLEDGMENTS**

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\(^{8}\)http://dao.mit.edu/~wen