doi:10.3969/j.issn.1001-4616.2017.03.016

Majorana Fermion in a System of One Dimensional Magnetic Atomic Chain

Yang Shuangbo

(Jiangsu Key Laboratory for NSLSCS,School of Physics and Technology,Nanjing Normal University,Nanjing 210023,China)

Abstract:For a model of one dimensional magnetic atomic chain in both a helical magnetic field and a transverse uniform magnetic field,we calculate its energy spectrum by solving Bogoliubov-de-Genes equation selfconsistently in the mean field approximation. We find that for a certain parameter setting,energy spectrum evolving with amplitude of helical magnetic field,appears Majorana fermion eigenstates. We calculate local density of states,and find that the local density of states for Majorana fermion shows peaks at the both ends(or at middle)of the magnetic atomic chain. We calculate wave function,and its spatial distribution agrees with local density of states.

Key words:Majorana fermion,magnetic atomic chain,BdG equation,localized density of states
CLC number:O413.1 **Document code**:A **Article ID**:1001-4616(2017)03-0110-08

一维磁性原子链系统中的 Majorana 费米子态

杨双波

(南京师范大学物理科学与技术学院,江苏省大规模复杂系统数值模拟重点实验室,江苏 南京 210023)

[**摘要**] 对处于螺旋形磁场及横向均匀磁场的一维磁性原子链模型,在平均场近似下通过自洽地求解 Bogoliubov-de-Genes 方程我们计算了系统的能谱. 我们发现在一定参数值的范围内能谱随螺旋形磁场振幅值演化呈现能量为零的 Majorana 费米子态. 我们计算了局域态密度发现对 Majorana 费米子其态密度的峰值出现在链的两端(或中点)位置. 我们计算了波函数其空间分布,发现它与局域态密度的结果一致.

[**关键词**] Majorana 费米子,磁性原子链,BdG 方程,局域态密度

Majorana fermion[1] which is a particle of the same as its own antiparticle, has been attracting great attention. Firstly,because of Majorana fermion being connected with topological phase concept,secondly because of its topological character,it provides a platform of potential application in topological quantum computing and quantum storing[2-4]. So experimentally and theoretically search for physical system of Majorana fermion has been a very hot research topic. The purpose of all these researches is to generate a topological superconductor,so that the Majorana fermion appears as a single excitation at the boundary.

Recently,Majorana fermion has been studied for a model of an atomic chain in a helical magnetic field in close proximity to a s-wave superconductor[5-7],and the result shows that at a certain parameter setting,the Majorana fermion is localized at the both end of the magnetic atomic chain. This is a spatially uniform system,after a gauge transformation,the Hamiltonian of the system will become an invariant form for space displacement. In this paper we modified this system by adding a new Zeeman term in the original Hamiltonian,which corresponds to a uniform magnetic field h perpendicular to the atomic chain being applied to the original system. Because of the new Zeeman term,the system is nonuniform spatially,we will study the structure of the Majorana fermion for the system of $h\neq 0$.

In this paper,we get the system eigenenergies and eigenvectors by numerically solving BdG equation,and then

Received data:2016-11-17.

Corresponding author:Yang Shuangbo,professor,majored in nonlinear physics and low dimensional system. E-mail:yangshuangbo@njnu.edu.cn

we study the birth and the localization in space of the Majorana fermion by calculating the spatially resolved local density of states and wave function. The structure of the paper is as the following,the Model and theory is in section 1,the result of numerical calculation and discussion is in section 2,the summary of the paper is in section 3.

1 Model and Theory

Consider a N-atom atomic chain in a helical magnetic filed or magnetic structure. The magnetic filed at site n is $\vec{B}_n = B_0(\cos n\theta \hat{e}_z + \sin n\theta \hat{e}_x)$, where θ is the angle made by the magnetic fields at the adjacent sites of the atomic chain,the whole atomic chain is in proximity to the surface of a s-wave superconductor,and in the transverse direction of the atomic chain a uniform magnetic field h is applied. The Hamiltonian of this magnetic atomic chain in mean field approximation is given by

$$H = t_x \sum_{n\alpha} (c^+_{n\alpha} c_{n+1\alpha} + h.c.) - \mu \sum_{n\alpha} c^+_{n\alpha} c_{n\alpha} + \sum_{n\alpha\beta} (\vec{B}_n \cdot \vec{\sigma})_{\alpha\beta} c^+_{n\alpha} c_{n\beta} + \sum_n \Delta(n)(c^+_{n\uparrow} c^+_{n\downarrow} + h.c.) + h \sum_{n\alpha} c^+_{n\alpha} (\sigma_z)_{\alpha\alpha} c_{n\alpha}, \quad (1)$$

where t_x is the jumping amplitude for electron between two adjacent sites,μ is chemical potential,$\Delta(n)$ is the superconductor pairing potential or order parameter at sit n,h is the weak uniform magnetic field for tuning system energy spectrum. $c^+_{n\alpha}$ or $c_{n\alpha}$ is the operator to creat or annihilate an electron of spin α respectively at site n,$\vec{\sigma}$ is pauli matrix vector,and $h.c.$ stand for complex conjugate. By introducing Nambu spinor representation $\psi_i = (c_{i\uparrow}, c_{i\downarrow}, c^+_{i\downarrow}, -c^+_{i\uparrow})^{\mathrm{T}}$,then Hamiltonian(1)can be written as BdG form,i.e. $H = \sum_{ij} \psi^+_i H_{ij} \psi_j$,where $\boldsymbol{H}_{ij}$ is the BdG Hamiltonian at site i,which can be written as

$$\boldsymbol{H}_{\mathrm{BdG}} = \begin{pmatrix} K_{ij} - \gamma_{ij} & B_0 \sin i\theta \delta_{ij} & \Delta(i)\delta_{ij} & 0 \\ B_0 \sin i\theta \delta_{ij} & K_{ij} + \gamma_{ij} & 0 & \Delta(i)\delta_{ij} \\ \Delta(i)\delta_{ij} & 0 & -K_{ij} - \gamma_{ij} & B_0 \sin i\theta \delta_{ij} \\ 0 & \Delta(i)\delta_{ij} & B_0 \sin i\theta \delta_{ij} & -K_{ij} + \gamma_{ij} \end{pmatrix}, \quad (2)$$

where $K_{ij} = t_x(\delta_{i+1,j} + \delta_{i-1,j}) - \mu\delta_{ij}$,$\gamma_{ij} = (h - B_0 \cos i\theta)\delta_{ij}$. This is a $4N \times 4N$ matrix,whose energy eigenvalue ε_n and eigenfunction $\boldsymbol{\psi}_n(i) = (u_n(\uparrow, i), u_n(\downarrow, i), v_n(\downarrow, i), v_n(\uparrow, i))^{\mathrm{T}}$, for $i = 1, 2, \cdots, N$,is determined by eigenvalue equation

$$\boldsymbol{H}_{\mathrm{BdG}} \boldsymbol{\psi}_n = \varepsilon_n \psi_n, \quad (3)$$

and boundary condition. In mean field approximation the order parameter at site i takes the form[8]

$$\Delta(i) = -U_0 \sum_{n, 0 < \varepsilon_n} \{ f_n [u_n(i,\uparrow) v^*_n(i,\downarrow) + u_n(i,\downarrow) v^*_n(i,\uparrow)] - \frac{1}{2} [u_n(i,\uparrow) v^*_n(i,\downarrow) + u_n(i,\downarrow) v^*_n(i,\uparrow)] \}, \quad (4)$$

and the mean number of electron at site i is

$$\langle n_i \rangle = \sum_\alpha \langle c^+_{i\alpha} c_{i\alpha} \rangle = \sum_{n, \varepsilon_n > 0} (|v_n(i,\uparrow)|^2 + |v_n(i,\downarrow)|^2) + \sum_{n, \varepsilon_n > 0} f_n [(|u_n(i,\uparrow)|^2 + |u_n(i,\downarrow)|^2) - (|v_n(i,\uparrow)|^2 + |v_n(i,\downarrow)|^2)], \quad (5)$$

where $f_n = 1/(1 + \mathrm{e}^{\varepsilon_n / k_{\mathrm{B}} T})$ is the Fermi distribution,T is temperature in Kelvin. The total number of electron is

$$N_t = \sum_{i=1}^{N} \langle n_i \rangle, \quad (6)$$

including spin up and spin down electrons. To determine eigenenergy,eigenfunction,order parameter,we need to selfconsistently solve eigenvalue equation(3)with(4)-(6). In this paper,we deal with the case of temperature $T = 0$,then the order parameter and the mean number of electron in site i are given by

$$\Delta(i) = (U_0/2) \sum_{n, 0 < \varepsilon_n} [u_n(i,\uparrow) v^*_n(i,\downarrow) + u_n(i,\downarrow) v^*_n(i,\uparrow)], \quad (7)$$

$$\langle n_i \rangle = \sum_{n, \varepsilon_n > 0} (|v_n(i,\uparrow)|^2 + |v_n(i,\downarrow)|^2). \quad (8)$$

Special case:$h = 0$ and $\Delta(i) = \Delta_0$,a constant. The Hamiltonian in(1)can be transformed into spatially unform

form by a gauge transformation. The topologically nontrivial region of the parameter set is given by

$$\sqrt{(|2t_x\cos(\theta/2)|-|\mu|)^2+\Delta_0^2}<B_0<\sqrt{(|2t_x\cos(\theta/2)|+|\mu|)^2+\Delta_0^2}, \tag{9}$$

where Majorana fermion corresponds to $\varepsilon_n=0$. As $|h|\neq 0$, Hamiltonian in(1) is nonuniform in space, and the nontrivial region of parameter set can not be obtained analytically.

In this paper we deal with open boundary condition with and without the middle magnetic domain wall, and at the magnetic domain wall we replace θ by $-\theta$. We have also studied under the periodic boundary condition, and found the result has no significant changes.

2 The Result of Numerical Calculation and Discussion

We first study the character of the Majorana fermion as the order parameter Δ and chemical potential μ are constants, then we study the influence of nonuniform $\Delta(i)$ on the result of Majorana fermion by doing selfconsistent calculation. In calculation, we choose the number of site N for the atomic chain according to the angle θ, so that the magnetic field at the both ends of the atomic chain points to the same direction.

2.1 Energy Spectrum and Wave Functions

For a one-dimensional magnetic atomic chain with magnetic domain wall in the middle, the parameter set is chosen as $\Delta_0=1.0, t_x=1.0, \mu=2.5, h=0.1, \theta=\pi/2$, and length of the chain is chosen as $N=81$ sites. For every value of B_0 in the interval $[1.0,4.0]$, we diagonalize the $4N\times 4N$ BdG Hamiltonian matrix(2), we get $4N$ energy eigenvalues and $4N$ eigenvectors. In open boundary condition, the energy spectrum is shown in Fig. 1. For B_0 in the interval $[1.486\,6, 3.996\,8]$, we can see that there exists eigenstates whose eigenenergy $\varepsilon_n=0$, and these eigenstates are Majorana fermions. The interval for the existense of Majorana fermion in the case of $h=0.1$ is very close to the interval $[1.476, 4.039]$ calculated from (9) for the $h=0$ case. For Majorana fermion at $B_0=2.1$, $\varepsilon_n=0$, shown in red dot in Fig. 1, we calculate its wave function $u_n(\uparrow,i), u_n(\downarrow,i), v_n(\uparrow,i), v_n(\downarrow,i)$, the result is shown in Fig. 2(a-d). We can see that the amplitude of the wave function concentrates on the both ends and the middle of the atomic chain. In Fig. 3, we show wave function for the same magnetic atomic chain without magnetic domain wall in the middle, the amplitude of the wave function concentrates on both ends of the magnetic atomic chain. This is similar to the previous result for the 1-dimensional magnetic atomic chain without uniform magnetic field, $h=0$.

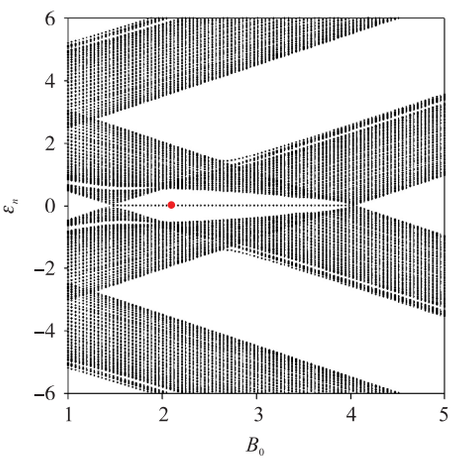


Fig. 1 The evolution of the energy spectrum with magnetic field amplitude B_0 for a one dimensional magnetic atomic chain with magnetic domain wall in the middle. The parameters are: $\Delta_0=1.0, t_x=1.0, \mu=2.5, h=0.1, \theta=\pi/2$, the length of the chain $N=81$

2.2 Local Density of States and Total Density of States

In this subsection, we study the space distribution of density of states(DOS), which is called local density of states(LDOS) and is defined as

$$\rho(\varepsilon,i)=\sum_{n,\sigma}|u_n(i,\sigma)|^2\delta(\varepsilon-\varepsilon_n)+|v_n(i,\sigma)|^2\delta(\varepsilon+\varepsilon_n)=$$
$$\sum_n[|u_n(i,\uparrow)|^2+|u_n(i,\downarrow)|^2]\delta(\varepsilon-\varepsilon_n)+[|v_n(i,\uparrow)|^2+|v_n(i,\downarrow)|^2]\delta(\varepsilon+\varepsilon_n), \tag{10}$$

$\rho(\varepsilon,i)$ is a function of energy and space position, and the total density of states(TDOS) can be written as

$$\rho_t(\varepsilon)=\frac{1}{N}\left[\sum_{n,\sigma,i}|u_n(i,\sigma)|^2\delta(\varepsilon-\varepsilon_n)+|v_n(i,\sigma)|^2\delta(\varepsilon+\varepsilon_n)\right], \tag{11}$$

i.e., the arithmetic mean of local density of states, a function of energy only. In numerical calculation, we

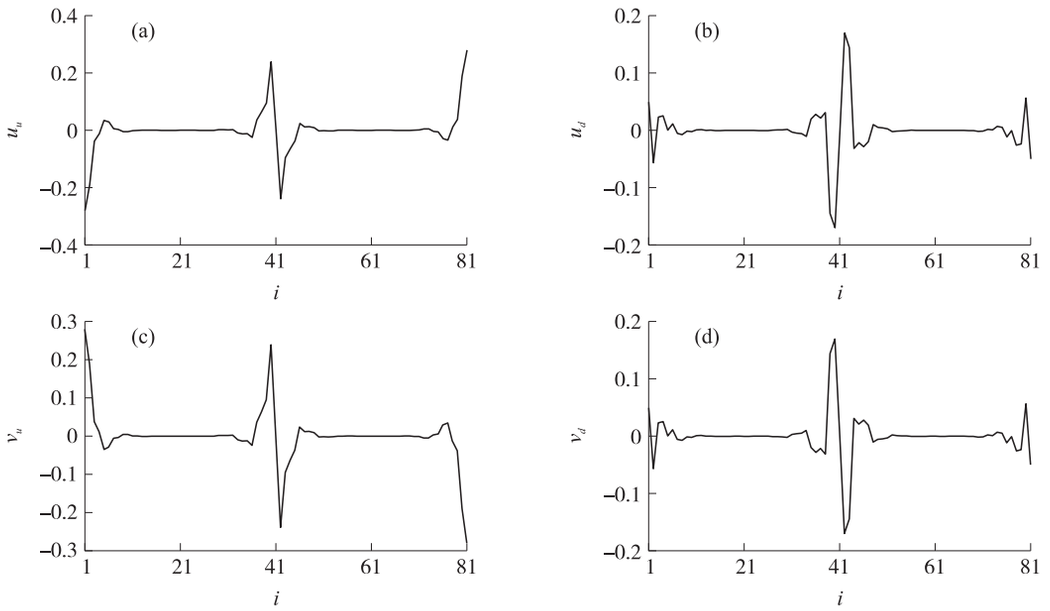


Fig. 2 Wave function of Majorana fermion for a magnetic atomic chain with a magnetic domian wall in the middle at $B_0=2.1$, and here $u(i,\uparrow)=u_u, u(i,\downarrow)=u_d, v(i,\uparrow)=v_u, v(i,\downarrow)=v_d$. The parameters are same as those shown in Fig. 1

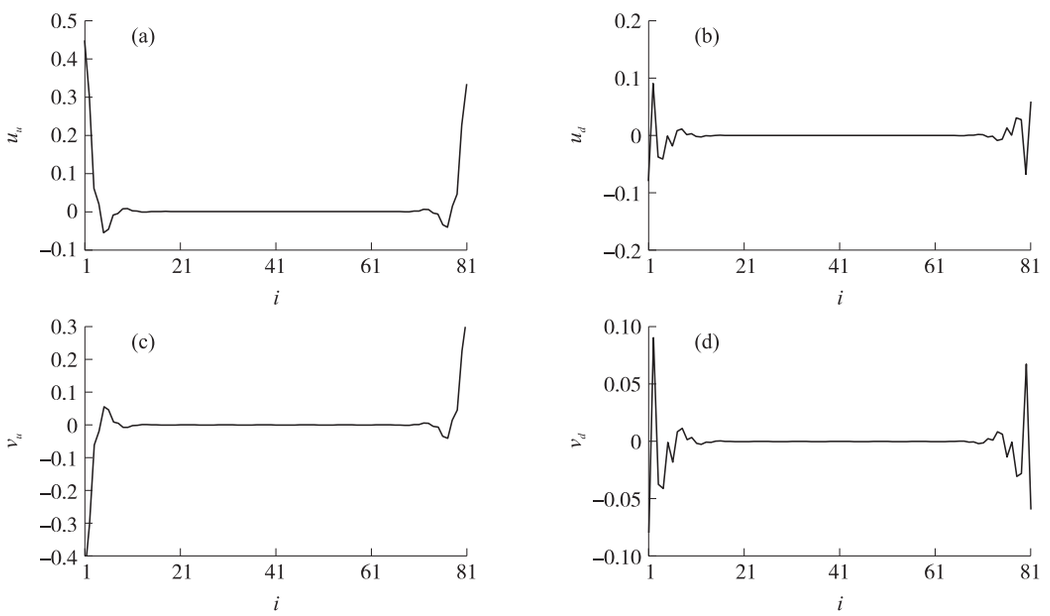
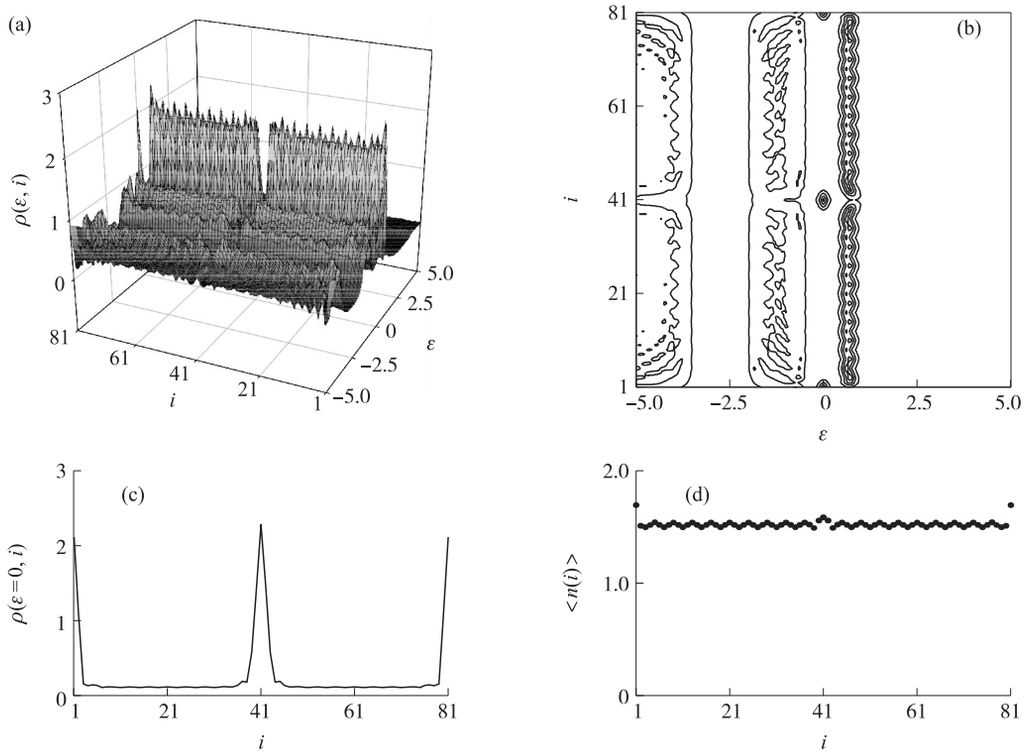


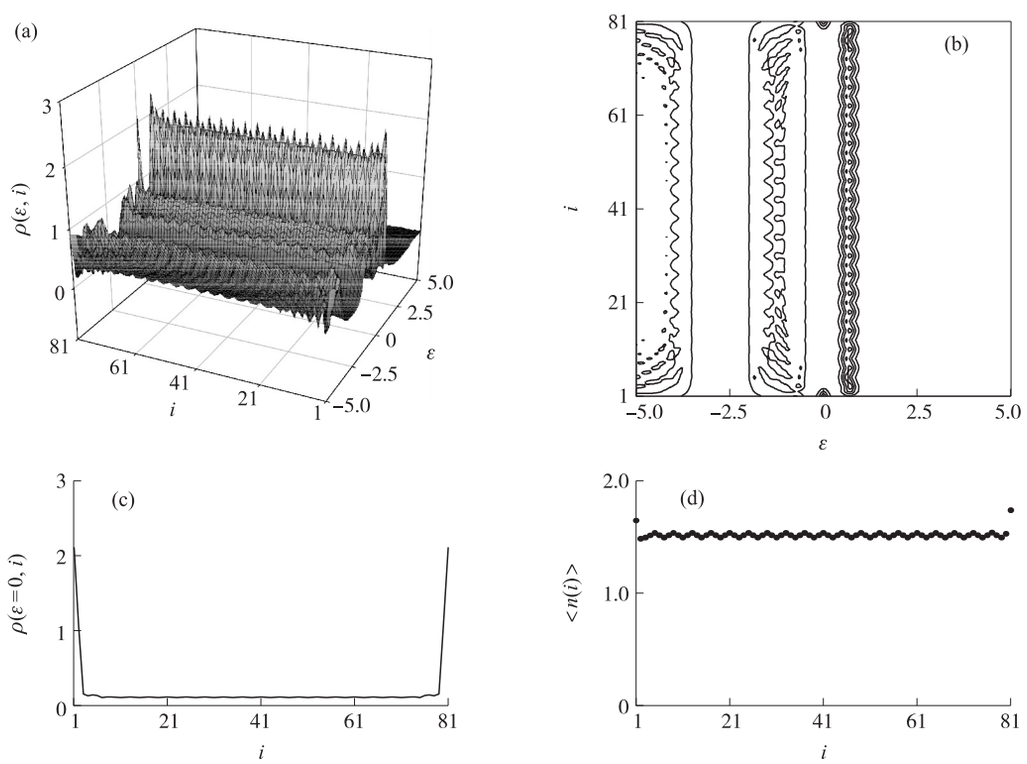
Fig. 3 Wave function of Majorana fermion for a magnetic atomic chain without a magnetic domain wall in the middle at $B_0=2.1$, and here $u(i,\uparrow)=u_u, u(i,\downarrow)=u_d, v(i,\uparrow)=v_u, v(i,\downarrow)=v_d$. The parameters are same as those shown in Fig. 1

replace δ by a Lorentz function. For parameter setting $h=0.1, t_x=1.0, \Delta=1.0, \mu=2.5, \theta=\pi/2, N=81$, and $B_0=2.1$, the local density of states for a Majorana fermion and the mean number of electrons on each site are shown in Fig. 4 (a–d) for the magnetic atomic chain with magnetic domain wall in the middle. Fig. 4(a) shows the local density of states $\rho(\varepsilon,i)$ in a 3D-plot; Fig. 4(b) shows the local density of states $\rho(\varepsilon,i)$ in a 2D contour plot; Fig. 4(c) shows the local density of states for Majorana fermion $\rho(\varepsilon=0,i)$; Fig. 4(d) shows the mean number of electron on each site of atomic chain $<n(i)>$. We can see from the Fig. 4 that the Majorana fermion is localized at two ends and middle for the magnetic atomic chain with magnetic domain wall in the middle. The mean number of electrons on each site of the atomic chain is around 1.5. In Fig. 5(a–d) we show the result for the same magnetic atomic chain without magnetic domain wall in the middle, then we see density of states for Majorana fermion is peaked only at both ends of the magnetic atomic chain.



(a)3D plot of the LDOS $\rho(\varepsilon,i)$;(b)2D contour plot of LDOS;(c)Distribution of LDOS for the Majorana fermion along the chain;(d) Average number of electrons on each site of the chain. The parameters are: $h=0.1$, $t_x=1.0$, $\Delta=1.0$, $\mu=2.5$, $\theta=\pi/2$, $N=81$, $B_0=2.1$.

Fig. 4　LDOS and average number of electrons on each site of the one dimensional magnetic atomic chain with the middle magnetic domain wall



(a)3D plot of the LDOS $\rho(\varepsilon,i)$;(b)2D contour plot of LDOS;(c)Distribution of LDOS for the Majorana fermion along the chain; (d)Average number of electrons on each site of the chain. The parameters are: $h=0.1$, $t_x=1.0$, $\Delta=1.0$, $\mu=2.5$, $\theta=\pi/2$, $N=81$, $B_0=2.1$.

Fig. 5　LDOS and average number of electrons on each site of the one dimensional magnetic atomic chain without the middle magnetic domain wall

2.3 The Self-consistent Result

As the order parameter $\Delta(i)$ is space position i dependent, we calculate the energy spectrum and local density of states by selfconsistently solving the eigenvalue equation(3) with equations(7) and(8). For parameter set $h=0.1, t_x=1.0, \mu=2.5, U_0=4.0, \theta=\pi/2, N=81$, the selfconsistently calculated energy spectrum is shown in Fig. 6, the Majorana fermion region can be seen, is still there, but the interval is shorten. The local density of states and mean numbers of electron on each site for Majorana fermion at $B_0=1.57$ are shown in Fig. 7(a-d) and Fig. 9(a-d). By comparison with Fig. 4(a-d), we find the main characters are same, but peak position for selfconsistent result moved inside a little bit. We calculate the selfconsistent wave function for Majorana fermion, and the results are shown in Fig. 8(a-d) and Fig. 10(a-d). The amplitude is significiently large at both ends for magnetic atomic chain without magnetic domain wall, and significiently large at both ends and middle for a magnetic chain with magnetic domain wall in the middle. This agrees with the result of local density of states.

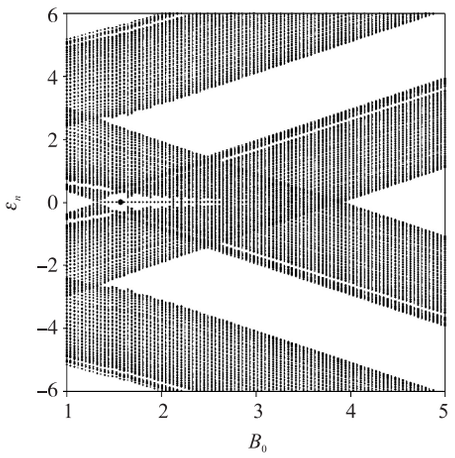
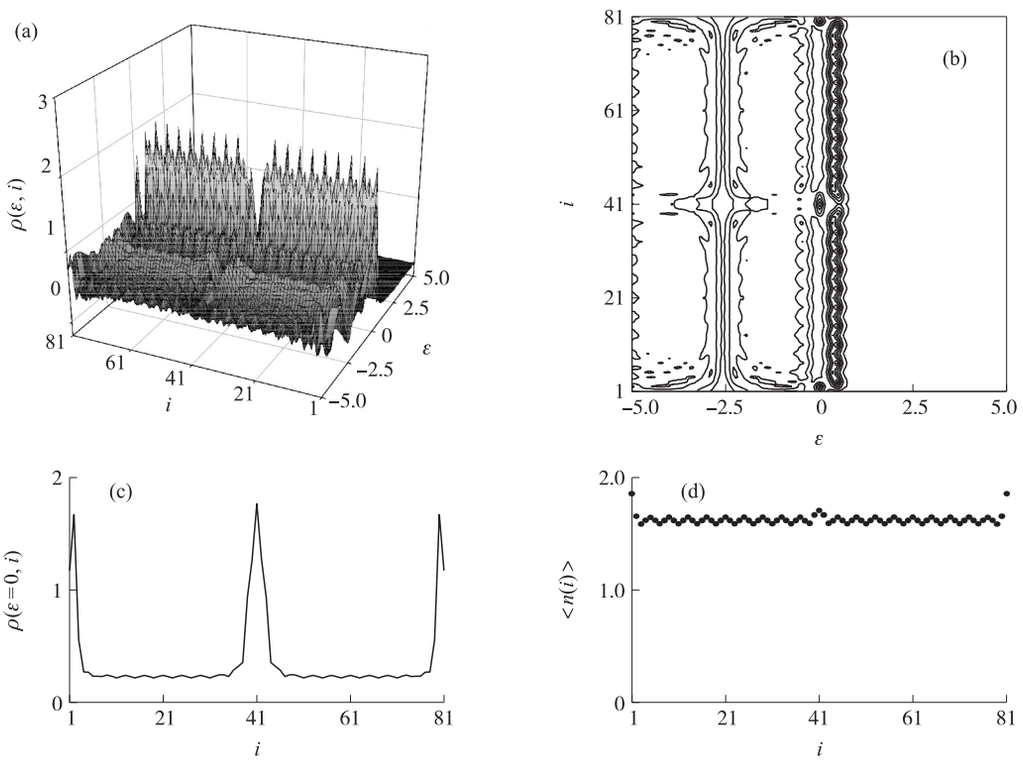


Fig. 6 The evolution of the selfconsistent energy spectrum with magnetic field amplitude B_0 for a one dimensional magnetic atomic chain with magnetic domain wall in the middle. The parameters are: $U_0=4.0, t_x=1.0, \mu=2.5, h=0.1$, $\theta=\pi/2$, and the length of the chain $N=81$



(a) 3D plot of the LDOS $\rho(\varepsilon, i)$; (b) 2D contour plot of LDOS $\rho(\varepsilon, i)$; (c) Distribution $\rho(\varepsilon=0, i)$ of LDOS for the Majorana fermion along the chain; (d) Average number of electrons on each site of the chain. The parameters are: $h=0.1, t_x=1.0, \mu=2.5, U_0=4.0, \theta=\pi/2, N=81, B_0=1.57$

Fig. 7 Selfconsistent LDOS and average number of electrons on each site of the one dimensional magnetic atomic chain with the middle magnetic domain wall

3 Summary

In mean field approximation, and by numerically solving Bogoliubov-de-Genes (BdG) equation, this paper

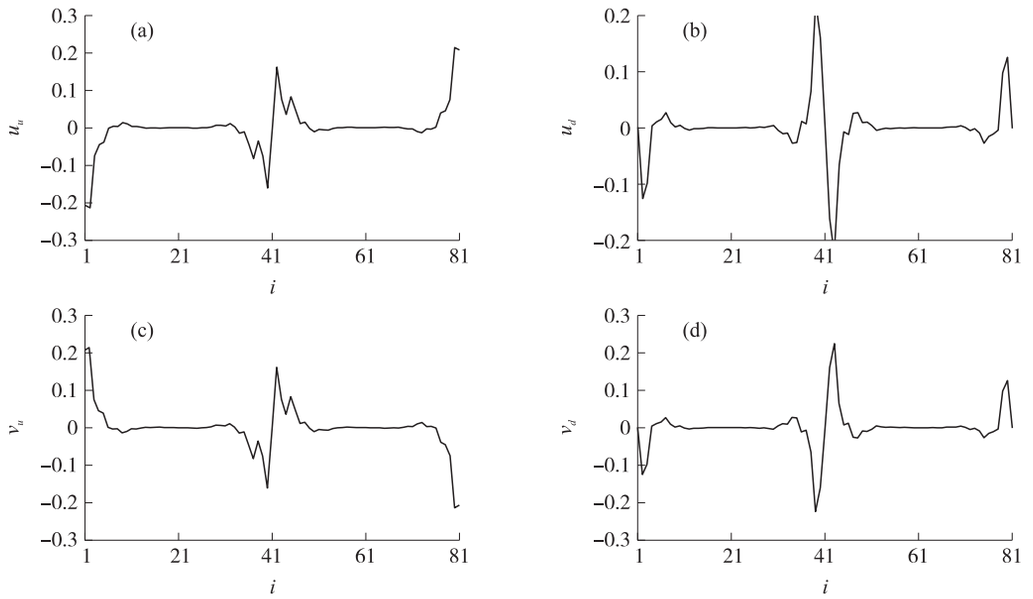
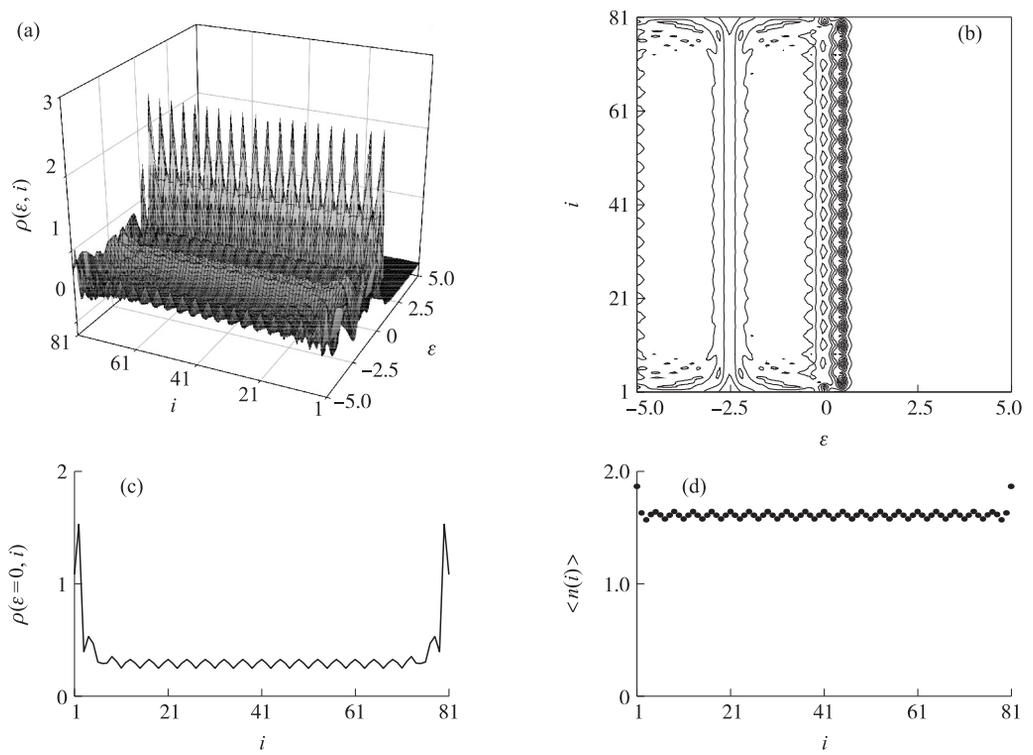


Fig. 8　Selfconsistent wave function for Majorana fermion for one dimensional magnetic atomic chain with the middle magnetic domain wall. Here $u(i,\uparrow)=u_u$, $u(i,\downarrow)=u_d$, $v(i,\uparrow)=v_u$, $v(i,\downarrow)=v_d$. The parameters are same as that in Fig. 7



(a) 3D plot of the LDOS $\rho(\varepsilon,i)$; (b) 2D contour plot of LDOS $\rho(\varepsilon,i)$; (c) Distribution $\rho(\varepsilon=0,i)$ of LDOS for the Majorana fermion along the chain; (d) Average number of electrons on each site of the chain. The parameters are: $h=0.1$, $t_x=1.0$, $\mu=2.5$, $U_0=4.0$, $\theta=\pi/2$, $N=81$, $B_0=1.57$

Fig. 9　Selfconsistent LDOS and average number of electrons on each site of the one dimensional magnetic atomic chain without a middle magnetic domain wall

studies the birth, and the localization in space of the Majorana fermion in a one dimensional atomic chain in helical magnetic field, and a uniform magnetic field h which is perpendicular to the atomic chain. Studies find that at a certain parameter setting, the evolution of the energy spectrum with helical magnetic field amplitude B_0 appears the zero energy eigenstates, which corresponding to the Majorana fermion. We calculate the local density of states, and find that the local density of states for the Majorana fermion has two peaks on the both end of the magnetic atomic

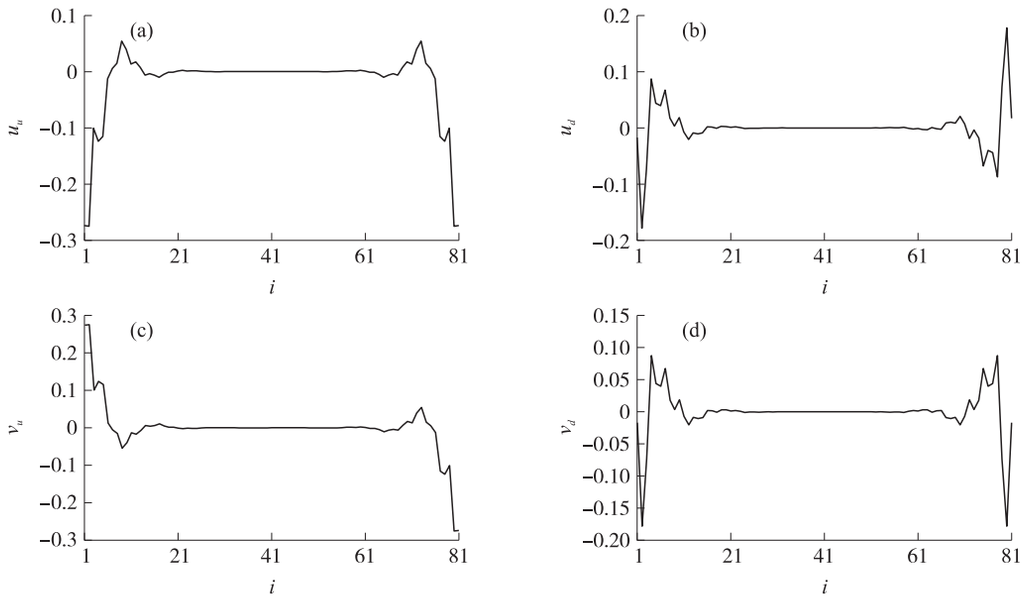


Fig. 10 Selfconsistent wave function for Majorana fermion for one dimensional magnetic atomic chain without a middle magnetic domain wall. Here $u(i,\uparrow)=u_u$, $u(i,\downarrow)=u_d$, $v(i,\uparrow)=v_u$, $v(i,\downarrow)=v_d$. The parameters are same as that in Fig. 9

chain. When a magnetic domain wall is applied at the middle of the maqgnetic atomic chain, the Majorana fermion shows peaks at both ends and the middle of the magnetic chain. As the order parameter is a function of space coordinate, we do selfconsistent calculation, and find that by comparing with the result of nonselfconsistent calculation, the energy spectrum and the shape of the local density of states are changed a little bit, but the main character does not change.

[参考文献]

[1] MAJORANA E. Symmetric theory of electron and positrons[J]. Nuovo Cimento, 1937, 14(1): 171-181.

[2] WILCZEK F. Majorana returns[J]. Nat Phys, 2009, 5(9): 614-618.

[3] NAYAK C, SIMON S H, STERN A, et al. Non-Abelian anyons and topological quantum computation[J]. Rev Mod Phys, 2008, 80(3): 1 083-1 159.

[4] ALICEA J. New directions in the persuit of Majorana fermions in solid state system[J]. Rep Prog Phys, 2012, 75(7): 076501-1-36.

[5] NADJ-PERGE S, DROZDOV I K, BERNEVIG B A, et al. Proposal for realizing Majorana fermions in chain of magnetic atoms on a superconductor [J]. Phys Rev B, 2013, 88(2): 020407-1-5(R).

[6] PÖYHÖNEN K, WESTSTRÖM A, RÖNTYNEN J, et al. Majorana state in helical shiba chain and ladders[J]. Phys Rev B, 2014, 89(11): 115109-1-7.

[7] VAZIFEH M M, FRANZ M. Self-organized topological state with Majorana fermions[J]. Phys Rev Lett, 2013, 111(20): 206802-1-5.

[8] SACRAMENTO P D, DUGAEV V K, VIEIRA V R. Magnetic impurities in a superconductors: effect of domainwall and interference[J]. Phys Rev B, 2007, 76(1): 014512-1-21.

[9] EBISU H, YADA K, KASAI H, et al. Odd frequency pairing in topological superconductivity in a one dimensional magnetic chain[J]. Phys Rev B, 2015, 91(5): 054518-1-15.

[责任编辑:顾晓天]