Numerical issues of two-dimentional Dirac equation

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The two-dimensional Dirac equation has been widely used in graphene physics, surface of topological insulators, and especially quantum scarring. Although a numerical approach to tackle an arbitrary confining problem was proposed several years ago, several fundamental issues needed to be thoroughly understood and solved. In this work, we conceal and address these challenges and finally develop a complete method, which is validated by comparison with analytical results.

I. INTRODUCTION

Two-dimensional Dirac equation has been widely use in graphene physics, surface of topological insulators and quantum scarring. As analytical methods such as boundary integral method [1] and conformal mapping method [2] could be used only to treat some specific case or failed to give both eigenvalues and eigenstates, it is of great interest to develop a numerical method that could solve two-dimensional Dirac equation confined in graphene physics, surface of topological insulators [5]. The Dirac equation is constrained in this domain and is 

\begin{equation}
\chi(x, y) = \psi(r, \varphi) \exp(i \theta_n),
\end{equation}

where \( \chi(x, y) \) represents respectively non-electric and electric potential, \( \mathbf{A} \) is the vector potential and \( \sigma_x, \sigma_y \) are Pauli matrices. The wave function is a 2-component spinor

\begin{equation}
\psi = (\phi, \chi)^T,
\end{equation}

whose elements are respectively positive and negative energy solutions.

There are many special features to this Hamiltonian. First, some symmetries are broken under certain conditions by considering the effects of antiunitary operators. What we are concerned about is that it breaks the parity symmetry. Denoting \( n \) th eigenfunction as \( \psi_n(x, y) \), it is evident that, when potentials are axial symmetric, \( \psi_n(x, y) \) does not necessarily satisfy \( H\psi_n(x, y) = \mu_n \psi_n(x, y) \) because of the existence of \( \alpha \) operator. However, in this case, \( |\phi_n(x, y)|^2 \) and \( |\chi_n(x, y)|^2 \) have parity [7].

Suppose we have an arbitrary domain \( D \), whose boundary is \( \partial D \) and the normal vector is denoted \( \mathbf{n} \). This domain can be simply-connected or multi-connected, which means it has many holes in the two-dimensional case. The Dirac equation is constrained in this domain and is described by the Hamiltonian mentioned in Section 2

\begin{equation}
H = \mathbf{A} \cdot (\mathbf{p} - eA) + m\sigma_z + U, \quad \mathbf{A} = (\sigma_x, \sigma_y), \quad r \in D
\end{equation}

with the boundary condition

\begin{equation}
\mathbf{j} \cdot \mathbf{n} = 0,
\end{equation}

where \( \mathbf{j} \) is the current vector. This boundary condition is equivalent to [1].

\begin{equation}
\chi/\phi = i e^{i \theta_n},
\end{equation}

where \( \theta_n \) is the angle of \( \mathbf{n} \).

It is difficult or even impossible to find a analytical solution for arbitray shape of \( D \), even if it is a rectangle. However, the analytical result for \( D \) being a unit circle exists and was given by [6]

\begin{equation}
\psi_{lm}(r, \phi) = N_{lm} \exp(i \phi) \left( J_l(\mu_{lm}r) \right),
\end{equation}

where \( N_{lm} \) is the normalization factor, \( J_l \) is the first order Bessel function and \( \mu_{lm} \) is the corresponding eigenvalue determined by the positive solution of

\begin{equation}
J_l(\mu_{lm}) = J_{l+1}(\mu_{lm}),
\end{equation}

which we will later use to validate numerical methods.

II. BACKGROUND

The general form 2 dimensional Dirac equation’s Hamiltonian is usually written as

\begin{equation}
H = \mathbf{A} \cdot (\mathbf{p} - q\mathbf{A}) + qU + \sigma_z V, \quad \mathbf{A} = (\sigma_x, \sigma_y),
\end{equation}

where \( V \) and \( U \) represent respectively non-electric and electric potential, \( \mathbf{A} \) is the vector potential and \( \sigma_x, \sigma_y, \sigma_z \) are Pauli matrices. The wave function is a 2-component spinor

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which we will later use to validate numerical methods.
Mathematically, we need $2N - 2M$ more equations to solve the equation set, which can be written as

$$B \Psi = 0,$$  \hspace{1cm} (10)

where $B$ is a matrix of $(2N - 2M) \times 2N$. Using these homogeneous equations, the question is reduced to

$$H_D \Psi_D = E \Psi_D$$  \hspace{1cm} (11)

where $\Psi_D$ is a column vector consisting of $2M$ independent variables.

An extra hermitization procedure is used by transforming $H_D$ to $H_D'$

$$H_D' = \frac{H_D + H_D^\dagger}{2}$$  \hspace{1cm} (12)

to prevent the eigenvalues from being complex [2]. However, we point out that this is not physical and would cause confusing results so that we won’t implement it here. The details are discussed in supplementary materials.

We call the method of using the vanishing current condition and the discretization above to study quantum scattering problems as vanishing current method (VCM) in the rest of the paper.

B. Problem of the Discretization scheme

Now we will prove that the discretization scheme above will result in incompleteness of equations. Suppose we have an arbitrary simply-connected domain $D$, and we build a mesh in Fig. (2). There are $m \times n$ unit cells in $G$, which in Fig 2 $m = 6, n = 6$. If $G$ takes the place of $D$, then it is evident that the numbers of variables, Dirac equations (a Dirac equation contributes two equations), and boundary equations are respectively $2(m+1)(n+1), 2mn, 2(m+n)$, which suggests the number of equations missing for completeness, denoted as $\Delta n$, satisfies

$$\Delta n = 2(m+1)(n+1) - 2mn - 2(m+n) = 2,$$  \hspace{1cm} (13)

which has nothing to do with the size of $G$ or the density of meshing.

Now let’s add some unit cells to domain $F$ to expand it, in a way that there will be no holes created nor go outside of $G$. After a unit cell is added, there will be one more Dirac equation, which corresponds to two equations. At the same time, we lose two boundary points, meaning the number of equations missing remains the same.

Finally, after enough unit cells are added, $F$ will overlap perfectly with $G$. Then, we can conclude that the number of equations missing for $F$ and $G$ is the same: two.

If we eliminate a unit cell inside $F$ to make one hole, we will lose one Dirac equation but gain four boundary
equations, subtracting $\Delta n$ by 2. Continuing to eliminate unit cells besides the first one, we will lose one Dirac equation but only gain two boundary equations, with $\Delta n$ uninfluenced. This indicate that if F has $t$ holes

$$\Delta n = 2 - 2t. \quad (14)$$

As long as the mesh is dense enough, the number of holes of F and D is the same. Besides, if there are some dangling inside D, those points that make F does not contain all of the inner points of D. There is one more spinor, which means two more variables, but only one boundary condition so that $\Delta n$ will be added by one. For arbitrary domain D, If the mesh is dense enough, there will be no dangling points. Therefore Eq. (14) is still applicable.

There is a lot of freedom in finding the extra boundary points when $n > 0$ or disqualifying some mesh points as boundary points when $n < 0$, which usually breaks the system’s symmetry if the potentials are symmetric and have a significant influence on the solution. When D has too many holes, which means $\Delta n \ll 0$, the impact of different choices is expected to be very large, while it is impossible to find the best general choice to minimize it.

We present a method where we don’t need to worry about the topology of the boundary. Note that an alternative way to simulate the impenetrable wall is the so-called mass-changing method, assuming the rest mass $m(r)$ is a position-dependent parameter and letting it go to infinity outside the domain. This method is widely used in the bag model of quark confinement. There is a misunderstanding that states one can either use the mass-changing method or boundary condition, as employed in VCM, to simulate the confinement [6]. As a closed system always has a boundary effect, it could not be eliminated like in periodic systems. Besides, similar to the incompleteness discussed above, the discretization scheme makes it impossible to write periodic boundary conditions completely.

Our solution is to combine the mass-changing method and zero current boundary condition. Berry’s boundary condition Eq. 4 is applied on $\partial K$ instead of $\partial D$, as shown in Fig. (2). All spinors in and on $\partial K$ are to be solved. The mass-changing method is introduced with a 4-scalar potential $V(r)$ that satisfies

$$V(r) = \begin{cases} +\infty & r \in K - D \\ 0 & r \in D \end{cases} \quad (15)$$

The domain $K - D$ could be simply or multi connected depending on the topology of D. But as K, a rectangular domain, is always simply-connected, as we proved above, we will always need two more equations regardless of the shape of D. Then we explain how to choose these 2 points so that we make its influence as small as possible. As $|\psi(r)|$ is predicted to be negligible where r is close to $\partial K$ because of the confinement, we can choose two extra 2 points at y axis, most relative to the top and bottom boundary, to preserve the mirror symmetry, which are points E1 and E2 in Fig. (2).

In practice, we replace $+\infty$ with a large positive number denoted as I. Here we estimate the suitable range of I as a function of the number of meshing elements in $x$ or $y$ direction denoted as N. The smoothed energy spectrum $\langle E(n) \rangle$ for infinite I is given by [1]

$$\langle E(n) \rangle \approx \sqrt{\frac{4\pi n}{S_D}}. \quad (16)$$

where $n$ is the energy level and $S_D$ is the area of D. For a finite I, we have $\langle E(n, I) \rangle > \sqrt{\frac{4\pi n}{S_D}}$. The total number of bounded states $n_{max}$ could be estimated by $\langle E(n_{max}, I) \rangle = I$ which gives $n_{max} < \frac{I^2 S_D}{4\pi}$. Due to our discretization method, we will get $n_0$ positive energy states given by

$$n_0 = N^2\frac{S_D}{S_K}, \quad (17)$$

where $S_K$ is the area K. The condition to approximate infinite high potential confinement is $n_0 \gg n_{max}$, which is reduced to

$$I \gg 2N\sqrt{\frac{\pi}{S_K}} \triangleq I_0. \quad (18)$$

However, as the discretized potential matrix is proportional to I, when it is too large, the other matrices’ contribution is lost and would lead to unphysical results. In other words, the confinement provided by the discretized zero current boundary condition is equal to a finite high

![Image](image-url)
potential $V_B(N)$, which tends to infinity when $N$ goes to infinity. $I$ should be much smaller than $V_B(N)$ to make the boundary condition valid. According to the practice, the range of $100I_0$ to $1000I_0$ is appropriate.

Besides, the size of the domain $K$–$D$ also matters. When it is too large, then we lose a lot of computational source to calculate the physics inside $D$. But if it is too small, the confinement might be affected since the wavefunction might be more easy to penetrate the potential wall. We show that actually the size of domain $K$–$D$ should be as small as possible. By selecting $D$ as a unit circle and $K$ as a square of diameter $2d$, we define $w$ as the difference between the radius of $K$ and $D$, i.e $w = d - 1$.

Then we measure the energy deviation from analytical results for different choices of $w$ in Fig. (3). The thinner the potential wall is, the limit of which is one element size, the more precise the result is. For general shape of $D$ without analytical results, this should also be true.

We name the new method as the mass changing and vanishing current method (MCVCM).

IV. RESULTS AND DISCUSSIONS

A. Comparing to analytical results

To compare the precision of MCVCM and VCM, we choose $D$, a unit circle domain, and $K$, a cubic domain with a diameter equal to 1, whose analytical eigenstates are given by Eq. (6) and Eq. (7). The result is shown in Fig. (4).

For eigenvalues, MCVCM has a 2% smaller relative error almost for all energy states considered, which is a huge difference for lower energy states. For eigenstates, VCM’s result tend to be uniform, which we interpret as a systematic problem of this discretization scheme. In contrast, MCVCM’s eigenvalues and eigenstates are closely consistent with the analytical ones and keep a good mirror symmetry and even some rotation symmetry imposed by the circular boundary.

B. Configuration for finite potential well

All of the discussions and results above are based on the confinement of a particle inside a wall of infinite potential. So it is natural to ask if our method, MCVCM, could be easily extended to the finite potential case. This problem is subtle. As we demonstrated before, the zero current boundary condition could not build valid infinite confinement that could both generates precise eigenstates and eigenvalues. In MCVCM, if we let the mass potential $V(r)$ be very small, then the results would tend to be that of VCM, where eigenstates become almost uniform, which is not physical. In other words, MCVCM fails to
simulate confinement induced by a small finite potential. We address this problem by adding an extra potential barrier $V'(r)$, which is very large, as illustrated in Fig. (5).

\[ V' \text{ is applied in the domain } K-X \text{ while } V \text{ is applied in the domain } X-D. \]

$V'(r)$ functions as a complement for the boundary condition. As discussed before, the domain K-X should be as small as possible to reach highest precision. If $V(r)$ is very small, the results won’t be affected by the systematic problem of the boundary condition confinement that gives closely uniform eigenstates. To evaluate the validity, we introduce two quantities defined as

\[ R = \int_D |\psi_n|^2 dS, \quad \text{IPR} = \int_K |\psi_n|^4 dS, \]

where $\psi_n$ is normalized by $\int_K |\psi_n|^2 dS = 1$. $R$ reflects the proportion of possibility density inside the $D$, which should tend to one as $V(r)$ goes higher. IPR describes the dispersion of eigenstate $\psi_n$. We take unit circle $D$ as an example, the results of which shown in Fig. (6). The existence of the extra barrier significantly raises $R$ and bring eigenstates away from being uniform when $V(r)$ is small.

\[ \text{FIG. 6. (a) is the mean value of } R \text{ and IPR for all bounded states as a function of } V. \text{ (b) and (c) are typical eigenstates of respectively MCVCM with extra barrer and MCVCM, for small potential.} \]

V. CONCLUSION

We have developed an refined method (MCVCM) and demonstrated it generates much more precise eigenvalues of eigenstates than VCM. First, we rigorously proved the incompleteness of equations and gave a solution where we don’t need to worry about the topology of the boundary. Second, we pointed out that under the discretization scheme in Section 2, a pure boundary condition is not enough to impose ideal confinement to the particle and would cause systematic errors. For more detailed discussion and application, check the supplementary materials.

Our work is expected to boost the research into the fields based on two-dimensional Dirac equation, such as graphene physics, topological insulators and quantum scarring.

[1] M. V. Berry and R. J. Mondragon, Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences 412, 53 (1987).
[2] H. Xu, L. Huang, Y.-C. Lai, and C. Grebogi, Physical Review Letters 110, 064102 (2013).
[3] J. Kogut and L. Susskind, Phys. Rev. D 11, 395 (1975).
[4] D. B. Kaplan, Physics Letters B 288, 342 (1992).
[5] R. Stacey, Physical Review D 26, 468 (1982).
[6] X. Ni, L. Huang, Y.-C. Lai, and C. Grebogi, Physical Review E 86, 016702 (2012).
[7] L. Huang, H.-Y. Xu, C. Grebogi, and Y.-C. Lai, Physics Reports 753, 1 (2018).
Supplementary Materials for

Numerical issues of two-dimensional Dirac equation

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1 Influence of different choices of extra boundary points

In MCVCM, there are always two extra boundary points which we should specify ourselves. In the main text, we briefly discussed about a optimal choice. Here we again choose a unit circle domain, comparing three different choices with analytical results, showing that this uncertainty does matter, especially related to breaking partial symmetry for high energy levels, as shown in Fig. (1).

2 Validity of zero current boundary condition for one-dimensional Dirac equation

To demonstrate it is valid to use zero current boundary condition for one-dimensional Dirac equation, we consider a massless particle confined in \([0, L]\) by infinite high potential at 0 and \(L\). The Hamiltonian and boundary condition is given by

\[
H = -i \partial_x \sigma_x, \quad H \psi(x) = E \psi(x), \quad j \cdot n = 0
\]  

(1)

The analytical solution for eigenvalues and eigenstates is given by

\[
\chi_n(x) = \sin(E_n x) - \cos(E_n x), \quad \phi_n(x) = -i \cos(E_n x) - i \sin(E_n x), \quad E_n = \frac{1}{2L} (2n - 1) \pi
\]  

(2)

We choose \(L = 1\) and compare the relative energy deviation and, especially, several low-energy eigenstates (both \(\chi\) and \(\xi\) components) with analytical results, as shown in Fig. (2). The method is the onedimensional version of VCM. Since the both the energy and eigenstates are close to analytical results, we conclude that VCM is valid when the dimension is one but fails when dimension is two as discussed in the main paper.

3 Influence of Hermitization

Physically, the Hamiltonian for a closed system should be Hermite. So it is natural to think it is also the case of the discretized Hamiltonian \(H_D\). However, the problem is not obvious as we used an unnormal discretization scheme to eliminate the fermion doubling effect. To evaluate the Hermicity of \(H_D\), the inner product of the ground state with all other states is used, as shown in Fig. (3). For VCM, \(|\langle \psi_n | \psi_1 \rangle|\) is large for almost all eigenstates. Therefore, hermitizied Hamiltonian \(\frac{H_D + H_D^\dagger}{2}\) differs a lot from non-hermitized \(H_D\), which is the reason for which the hermitization procedure is not physical and would not generate precise results.

S1
Figure 1: Energy deviation of MCVCM by different choices of extra boundary points (a). The mesh number $N$ is 80. Some typical high energy states for these choices are plotted in (b, c) at the energy level of 400. The green solid circles are rough places where the extra boundary points are sampled.
Figure 2: Relative energy deviation \((a)\) and several eigenstates for massless Dirac particle confined in \([0, 1]\). \((b1)\) and \((b2)\) are \(|\phi|\) for the lowest two states; \((b3)\) and \((b4)\) are \(|\chi|\) for the lowest two states. The number of mesh elements is 1000. The red and blue line are respectively analytical and numerical result.
For MCVCM, \(|\langle \psi_n | \psi_1 \rangle|\) is small for the former 4000 states, which are bounded states with energy lower than the mass potential. This is expected as the low energy states are consistent with the analytical results shown in the main text. While for the scattering states, it is relatively large, indicating the orthogonality of scattering states and bounded states are weak. Therefore, we can’t apply hermitization on MCVCM either because of this distinct inconformity of the orthogonality of bounded and scattering states.

![Figure 3: Picture to show the preservation of hermicity of MCVCM and VCM. The boundary is a unit circle, and each direction’s meshing number \(N\) is 80. Because VCM only computes points inside the boundary, the total number of states is less than that of MCVCM.](image)

4 Relativistic quantum scarring

4.1 Chiral scar and its control

By now, only the conformal mapping method has been used to demonstrate chiral scar in closed systems for some unique shapes where such a map could be found to transform the solution from a unit circle, like heart and African shape\[.\] However, the limit is that if an arbitrary shape is given, it is usually very difficult or even impossible to find a conformal mapping for it, especially for the boundary of a multi-connected domain.

Besides, a small circular hole in the center is needed to exclude the magnetic field from the physical domain, which should also tend to zero to get the analytical results. However, due to experimental limits, the size of the hole is always finite, whose shape should also be changeable regardless of the shape of the domain \(D\). Therefore, it remains an open question if the control of chirality described by the semiclassical theory \[? \] is still valid when the hole is finite small and arbitrary shape.

Since scars exist only in high energy levels, it impose a strong requirement on the precision of the numerical method. Even for MCVCM, the relative energy deviation from analytical results for unit
circle is up to 50% for energy levels highest to 2000. And due to the huge computational cost, it is hard to raise the precision under current capability of computers. Nevertheless, we still observe scars in high energy levels despite the inaccuracy and managed to tune chirality by magnetic field.

We chose the external boundary of D as a playground, which could not be solved using the conformal mapping method. Then we choose two different holes, an eclipse hole with the major axis of 0.3 and the minor axis of 0.5 and a circular hole with a radius of 0.3. Without losing generality, we let $e = 1$. The vector potential is given by

$$ A(r, \phi) = \alpha \left( \frac{-\sin \phi}{r}, \frac{\cos \phi}{r} \right), $$

where $\alpha$ is called the flux parameter. This vector potential is to generate a singular magnetic field at origin

$$ B = \nabla \times A = 2\pi \alpha \delta(r) \hat{z}. $$

As a result, for any circuit $C$ about the hole, the wave function will acquire a phasor factor

$$ \varphi' = \exp \left[ -i \oint_C A \cdot dr \right] \varphi = \exp(-2i\alpha \pi W_C) \varphi, $$

where $W_C(= \pm 1)$ is the winding number of $C$. For a clockwise and counterclockwise scar orbit, the phase difference due to magnetic field is $-4\pi \alpha$. Due to spin-boundary interaction, the phase difference between reversed scars of odd bouncing numbers will be $\pi$ while that for even bouncing numbers is 0 (mod $2\pi$). The former kind is called the chiral scar. Phenomenologically, these two kinds of phase change could be included in the semiclassical formulas

$$ \Delta \Phi = kL + 2\pi W_C \alpha - \sigma \pi \frac{\pi}{2} + 2\pi \beta, $$

where $k$ is the energy level of the scar and $L$ is the orbit circumference. $\sigma$ is the Maslov index which on this occasion is equal to the bouncing number. $2\pi \beta$ is the phase shift caused by the spin-boundary interaction that differs by $\pi$ for scars of odd bouncing numbers. For semiclassical allowed orbits, $\Delta \Phi = 2\pi n (1, 2, \cdots)$ to ensure the wavefunction is single-valued. This result in non-chiral scars of the same pattern reoccurring at an energy difference of $\delta k = \frac{2\pi}{L}$ while for chiral scars $\delta k = \frac{\pi}{L}$. When $\alpha = 0.25$ is satisfied, the corresponding scar will switch from chiral to non-chiral or vice-versa.

Here we consider scars in the shape of a rectangle, which is non-chiral. We define $\eta$

$$ \eta(n) = \{ \frac{k_n - k_{n-1}}{k_0} \}, \quad k_0 = \frac{2\pi}{L} $$

where $k_{n-1}$ and $k_n$ are two adjacent energies where rectangular scar appears and {} represents the decimal part of a number. For chiral scars, $\eta(n)$ is predicted to be around zero or one. For non-chiral scars it should be around 0.5. We tested $\alpha = 0, \alpha = 0.25$ to show the control of chirality in Fig (4). Due to numerical precision and the relative low energy level, $\eta$ could be around 0.5 in some circumstances. We expect the it to be more close to the semiclassical theory in the future when we have more powerful computational capability.
Figure 4: Illustration of control of chirality. The scars are chosen in the energy level 1000 to 2000. (a) and (c) show the scars outlined by blue strokes for two different shapes of holes. The corresponding $k_0$ is 0.685. The yellow circle in center represents Aharonov–Bohm flux. $\eta(n)$ and its fitted density distribution $f_S(\eta)$ are shown in (b,d).
5 Possible higher order discretization scheme

The current discretization scheme is based on the finite differential formula to the first order

\[ f'(x) \approx \frac{f(x + a) - f(x - a)}{2a} \]  

(8)

Extending it to the second order we have

\[ f'(x) = \frac{2}{3a}[f(x + a) - f(x - a)] - \frac{1}{12a}[f(x + 2a) - f(x - 2a)]. \]  

(9)

Similarly, one could develop a higher order discretization scheme compatible with eliminating fermion doubling effect as follows

\[ \partial_x f_{m+\frac{1}{2},n+\frac{1}{2}} = \frac{2}{3h_x}[f_{m+1,n+1} + f_{m+1,n} - f_{m,n} - f_{m,n+1}] - \frac{1}{12h_x}[f_{m+2,n+1} + f_{m+2,n} - f_{m-1,n} - f_{m-1,n+1}], \]

\[ \partial_y f_{m+\frac{1}{2},n+\frac{1}{2}} = \frac{2}{3h_y}[f_{m+1,n+1} + f_{m,n+1} - f_{m,n} - f_{m+1,n}] - \frac{1}{12h_y}[f_{m+1,n+2} + f_{m,n+2} - f_{m,n-1} - f_{m+1,n-1}], \]

\[ f_{m+\frac{1}{2},n+\frac{1}{2}} = \frac{1}{4}(f_{m,n} + f_{m+1,n} + f_{m,n+1} + f_{m+1,n+1}). \]  

(10)

Then we tested the results for the first order discretization scheme in the paper and the second order discretization scheme above with analytical results for unit circle boundary as shown in Fig. (5). The high deviation of low energy states calculated by the second order method implies its failure. But it is possible to adjust

\[ f_{m+\frac{1}{2},n+\frac{1}{2}} = \frac{1}{4}(f_{m,n} + f_{m+1,n} + f_{m,n+1} + f_{m+1,n+1}) \]  

(11)

to relate more points in order to raise the precision.
Figure 5: Relative energy deviation $\Delta E/E$ for first and second order discretization scheme of MCVCM (a) and energy level for the above two numerical methods and analytical results (b). The blue line and red line, respectively in each subfigure, represent second order and first order discretization scheme of MCVCM. The yellow line in (b) represents the analytical result.