

Spin-Charge Separation in Two Dimensions: A Numerical Study

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Abstract

The question of spin-charge separation in two-dimensional lattices has been addressed by numerical simulations of the motion of one hole in a half-filled band. The calculations have been performed on finite clusters with Hubbard and t - J models. By comparing the time evolution of spin and charge polarisation currents in one and two dimensions, evidence in favor of spin-charge separation in two dimensions is presented. In contrast with this, spin-charge separation is absent in a highly doped, metallic, system.

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The crucial issue in understanding the physics of strongly-correlated systems is the nature of the ground state and low-lying excitation the normal state of doped high- T_c materials. In particular, intense attention has been focused on the question of spin-charge separation and non-Fermi (or Luttinger) liquid behaviour of Hubbard and related models in 2D. It has been forcefully argued by Anderson [1] that the breakdown of Fermi liquid behaviour and the phenomenon of spin-charge separation, well established in 1D, is carried over to 2D systems and weakly coupled chains and planes as well. These arguments are substantiated by physically motivated scattering theory and anomalous fermionic backflow [2] calculations. The interlayer tunneling mechanism proposed by Wheatley, Hsu, and Anderson [3,4] crucially depends on the existence of spin-charge decoupled layers coupled via a weak interlayer hopping term. However, in spite of extensive investigations, both analytical and numerical, so far there is no clear, convincing signature of non-Fermi liquid behaviour in 2D.

The situation in 1D is clearer due to the exact solutions of Hubbard [5] and Tomonaga-Luttinger models and other calculations. [6] The physics in 1D, in the absence of a magnetic field, is characterized by three parameters, which are u_ρ (charge velocity), u_σ (spin velocity), and K_ρ (coefficient that determines the long range decay of correlation functions). u_ρ and u_σ , in the large- U limit, are, respectively, given by $2t \sin \pi n$ and $\frac{2\pi t^2}{U}(1 - \frac{\sin 2\pi n}{2\pi n})$ where t, U are the Hubbard model parameters and n is the particle density ($n \leq 1$). This physics is described in terms of spinons (excitations carrying spin-1/2 but no charge) and holons (excitations carrying unit charge but no spin), and implies that the two kinds of excitations have altogether different dynamics. This is called spin-charge separation.

Thus in the case of 1D, the non-Fermi liquid behaviour typically manifests itself as (i) the power-law behaviour of correlation functions; in particular, of the momentum distribution around \mathbf{k}_F , and (ii) spin-charge separation. Away from 1D, the only exact results available are due to Fabrizio and Parola [7] on coupled chains with a modified Tomonaga-Luttinger model, in which case spin-charge separation is shown to exist. On the other hand, calculations which *do not* observe spin-charge separation in coupled chains, are quite numerous. [8] Numerical attempts, in 2D, as regards the power-law behaviour of the momentum distribu-

tion are inconclusive. [9] In this work, we prefer to focus our attention on the possibility of observing spin-charge separation by simulating the motion of one hole in a half-filled band. Indeed, we do demonstrate spin-charge separation in 1D, and by comparing the behaviour seen in 2D with that in 1D, present a favourable evidence for such a separation in 2D.

Now we describe the simulation procedure. We introduce a Gaussian hole, at time $t = 0$, into the ground state $|G\rangle$ of a cluster, Hubbard or t - J , at half-filling, obtained by exact diagonalization. [4,10] The resulting state can be written as

$$|\psi(0)\rangle = \sum_i e^{i\mathbf{K}_0 \cdot (\mathbf{r}_i - \mathbf{R}_0) - \beta |\mathbf{r}_i - \mathbf{R}_0|^2} c_{i\sigma} |G\rangle. \quad (1)$$

The charge distribution at $t = 0$ is centered around \mathbf{K}_0 in momentum space with spread $\sim \sqrt{\beta}$ and \mathbf{R}_0 in real space with spread $\sim \frac{1}{\sqrt{\beta}}$. This state is then subjected to (second-order) time evolution

$$|\psi(t + \Delta t)\rangle = (1 - i\Delta t H - \frac{1}{2}(\Delta t H)^2)|\psi(t)\rangle, \quad (2)$$

during which various quantities pertaining to charge and spin are computed. It is well known that the finite time step (and the approximate form for the time evolution operator) tends to make the evolution nonconservative. This error can only be reduced by using a small enough time step and by including higher-order terms in the time evolution operator, which is the reason for using the second-order form rather than the (numerically less costly) first-order one. Further, the time step is chosen to ensure that the energy expectation value in the state $|\psi(t)\rangle$ always remains within a few percents of its initial value. This procedure is indeed the same as that of Jagla *et al.*, [11] except that we are using the second-order approximation to the time evolution operator. They demonstrated that spin-charge separation can readily be observed on small 1D clusters by numerical means. They failed to see it in 2D because of very high doping. This point will be discussed later. The “visual” results of their paper in 1D have been confirmed by us.

In order to find an appropriate quantity that would reflect spin-charge separation, let us recall that spin-charge separation results from the dynamical independence of spin and

charge degrees of freedom, which should be reflected in the dynamical behaviour of charge (+) and spin (−) densities:

$$\rho_{\pm}(i, t) = \frac{\langle \psi(t) | (n_{i\uparrow} \pm n_{i\downarrow}) | \psi(t) \rangle - B_{\pm}}{\sum_i (\langle \psi(0) | (n_{i\uparrow} \pm n_{i\downarrow}) | \psi(0) \rangle - B_{\pm})}. \quad (3)$$

Here B_+ is the average background charge (number of electrons per site, = 1 for the half-filled ground state) and B_- is the average background spin (= 0 for the half-filled ground state belonging to the $S_z = 0$ subspace). These are thus the densities associated with the doped particle, and are normalized to unity. In the non-interacting ($U = 0$) case, we expect $\rho_+(i, t)$ to vary in time identically as $\rho_-(i, t)$, whereas in the spin-charge decoupled case, these two quantities should show a non-trivially different behaviour in time. It is more convenient to define site-independent aggregate quantities from these, which are polarisations [12]

$$\mathbf{P}_{\pm}(t) = \sum_i \mathbf{r}_i \rho_{\pm}(i, t). \quad (4)$$

Qualitatively, the polarisations reflect the center-of-mass movement of the charge and spin peaks. Since they are origin-dependent, we prefer to look at their rates of change, $\frac{d\mathbf{P}_{\pm}(t)}{dt}$, which are the average classical currents set up in the system due to the time evolution of the hole packet, and are a measure of charge and spin group velocities. [13]

We have carried out extensive simulations on the following 1D and 2D clusters: (i) six-site Hubbard ring, (ii) (4+4) site coupled Hubbard chains, (iii) 4×4 t - J plane, with one hole doped in the half-filled ground state, and (iv) 4×4 Hubbard plane with one *extra electron* in the two-electron ($S_z = 0$) ground state. Periodic boundary conditions have been used in all the cases. Note that the t - J model has been used only in the case where it is impossible to work with the Hubbard model due to the large-basis problem. This, we think, is acceptable, since we believe that the essential physics of the large- U Hubbard model is contained in the $t - J$ model. Simulations are done by varying the width of the Gaussian, β , and for all \mathbf{K}_0 appropriate for a given cluster, as well as the model parameters U or J .

We first present the results on the 1D six-site ring, for which spin-charge separation is known to exist. These will bring out the characteristic behaviour of currents $\frac{d\mathbf{P}_{\pm}(t)}{dt}$ in the

spin-charge separated case as against the noninteracting, undecoupled case. For all these runs, we choose $\beta = 0.1$ and $\mathbf{K}_o = \frac{-2\pi}{3}$. All energies and times are measured with respect to the Hubbard parameter $t = 1$. Figure 1 shows the currents as a function of time (up to 2000 steps, $\Delta t = 0.01$) for values of $U = 0$ [Fig. 1(a)], $U = 1$ [Fig. 1(b)] and $U = 20$ [Fig. 1(c)]. As expected, for the noninteracting case [Fig. 1(a)], the two curves overlap for all times, and show a periodic behaviour characteristic of the free motion of a hole packet on a periodic lattice. This also means that $\rho_{\pm}(i, t)$, at each site i , oscillates with the same frequency. As U increases [Fig. 1(b)], the charge and spin currents start “separating,” indicating the response of the background, although the periodicity of the $U = 0$ case is still evident, including the locations of the peaks. However, the behaviour of $\frac{d\mathbf{P}_+}{dt}$ and $\frac{d\mathbf{P}_-}{dt}$ are dramatically different from each other for large U , beyond $U \sim 5$, indicating the decoupling of spin and charge dynamics [Fig. 1(c)]. The contrast between Fig. 1(b) and 1(c) can be related to the “stiffening” of the antiferromagnetic background with increasing U . In order to understand the highly oscillatory behaviour of the currents, let us note that by creating a hole at $t = 0$ in the background (i.e., half-filled ground state), we have created a state that is *not* an eigenstate of the system, and can be written as a linear combination of ground and excited states. In 1D, these excited states can always be described [6] as spinon and holon excitations, having different dynamics, and we believe that the observed behaviour of the currents in Fig. 1(c) is a direct consequence of this.

Now we present the results for the 2D system (4×4 t - J cluster). For this case we choose $\mathbf{K}_0 = (\frac{-\pi}{2}, \frac{-\pi}{2})$, $\beta = 1$, and $J = 0.1$. The initial Gaussian hole packet has been placed symmetrically with respect to the entire lattice, because of which the y component of the currents varies identically as the x component, for this \mathbf{K}_0 . [14] We thus display, in Fig. 2, only the x components of spin and charge currents. Clearly, the two currents indicate different dynamics, in that, their magnitudes as well as directions (and phases) are different from each other almost all the time. This feature is qualitatively similar to Fig. 1(c) for the 1D case, $U = 20$. We interpret this as a signature of spin-charge separation in 2D. Qualitatively similar behaviour is seen for J as large as 0.8, which is not surprising,

since the t - J model has strong correlations built-in because of the elimination of double occupancy, throughout the parameter range.

It is to be noted that the above mentioned behaviour is observed for *one* hole doped into the half-filled ground state of the 4×4 cluster. In order to show that this behaviour, indicative of spin-charge separation, *does not* persist for high doping—the metallic case, we examine the time evolution of one *extra electron* in the two-electron ($S_z = 0$) ground state of the 4×4 Hubbard cluster as a function of U . We have $\beta = 1.0$, $\mathbf{K}_0 = (\frac{-\pi}{2}, 0)$ and the gaussian packet is again placed symmetrically with respect to the lattice. There is no current in the y direction because of this choice of \mathbf{K}_0 and \mathbf{R}_0 [14]. Fig. 3 (a) and (b) depict the x currents for $U = 0.1$ and $U = 10$ respectively. Indeed, it is observed that the familiar periodic behaviour (with more or less overlapping curves), indicative of a weakly interacting, spin-charge *undecoupled* system, is observed even for U as high as 10. This is precisely the reason why Jagla *et al.* [11] did not observe spin-charge separation in their study in 2D.

In conclusion, we have studied numerically the time evolution of one hole in a half-filled band, and by comparing the behaviour of spin and charge currents in 2D with that in 1D, we have presented evidence in favour of spin-charge separation in 2D lattices. We have also demonstrated that this phenomenon is observed only in the low-doped systems (one hole in the present case) and is absent in the high-doping limit (low electron densities). Finally, we note that our calculations on $4 + 4$ coupled chains (not presented here) also display a similar behaviour which is indicative of spin-charge separation in coupled systems.

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- [13] In the 1D case, these currents are not related, in any simple way, to the 1D expressions

for charge and spin velocities $u_\rho = 2t \sin \pi n$ and $u_\sigma = \frac{2\pi t^2}{U} (1 - \frac{\sin 2\pi n}{2\pi n})$, because the state that we obtain on doping is *not* an eigenstate of the system, whereas u_ρ and u_σ have been obtained from the *exact* excitation spectrum as group velocities of charge and spin excitations in the limit of zero momentum: see C. F. Coll, Phys. Rev. B **9**, 2150 (1974).

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Figure Captions

FIG. 1 Currents $\frac{d\mathbf{P}_{\pm}(t)}{dt}$ as functions of time for one hole in the half-filled ground state of the six-site Hubbard ring for different values of U : (a) $U = 0$, (b) $U = 1$, (c) $U = 20$; solid curve, charge current; dotted curve, spin current.

FIG. 2 x components of currents $\frac{d\mathbf{P}_{\pm}(t)}{dt}$ as functions of time for one hole in the half-filled ground state of the (4×4) -site t - J cluster; solid curve, charge current; dotted curve, spin current.

FIG. 3 x components of currents $\frac{d\mathbf{P}_{\pm}(t)}{dt}$ as functions of time for one extra electron in the two-electron ground state of the (4×4) -site Hubbard cluster for different values of U : (a) $U = 0.1$, (b) $U = 10$; solid curve, charge current; dotted curve, spin current.

Fig. 1(a)

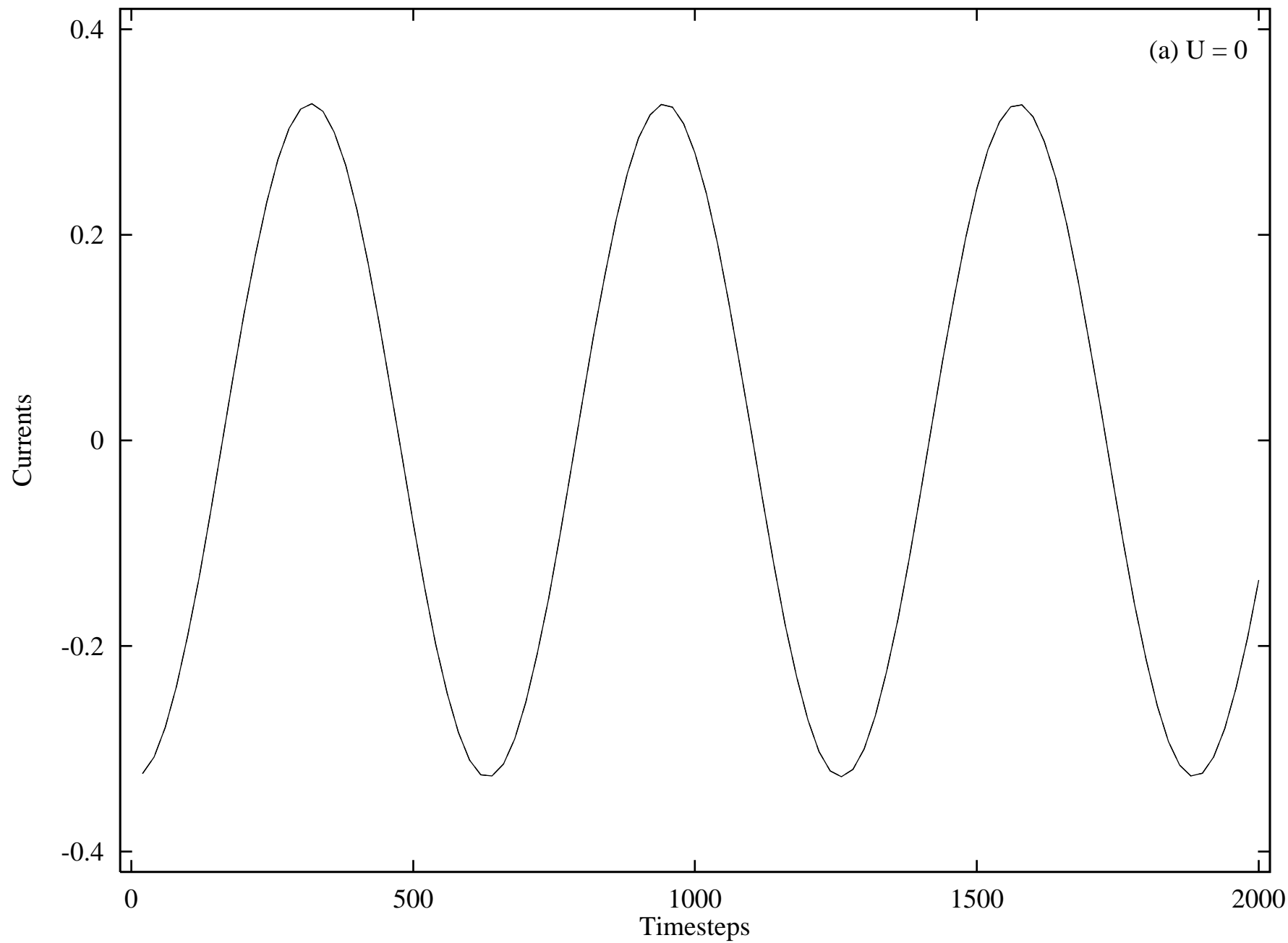


Fig. 1(b)

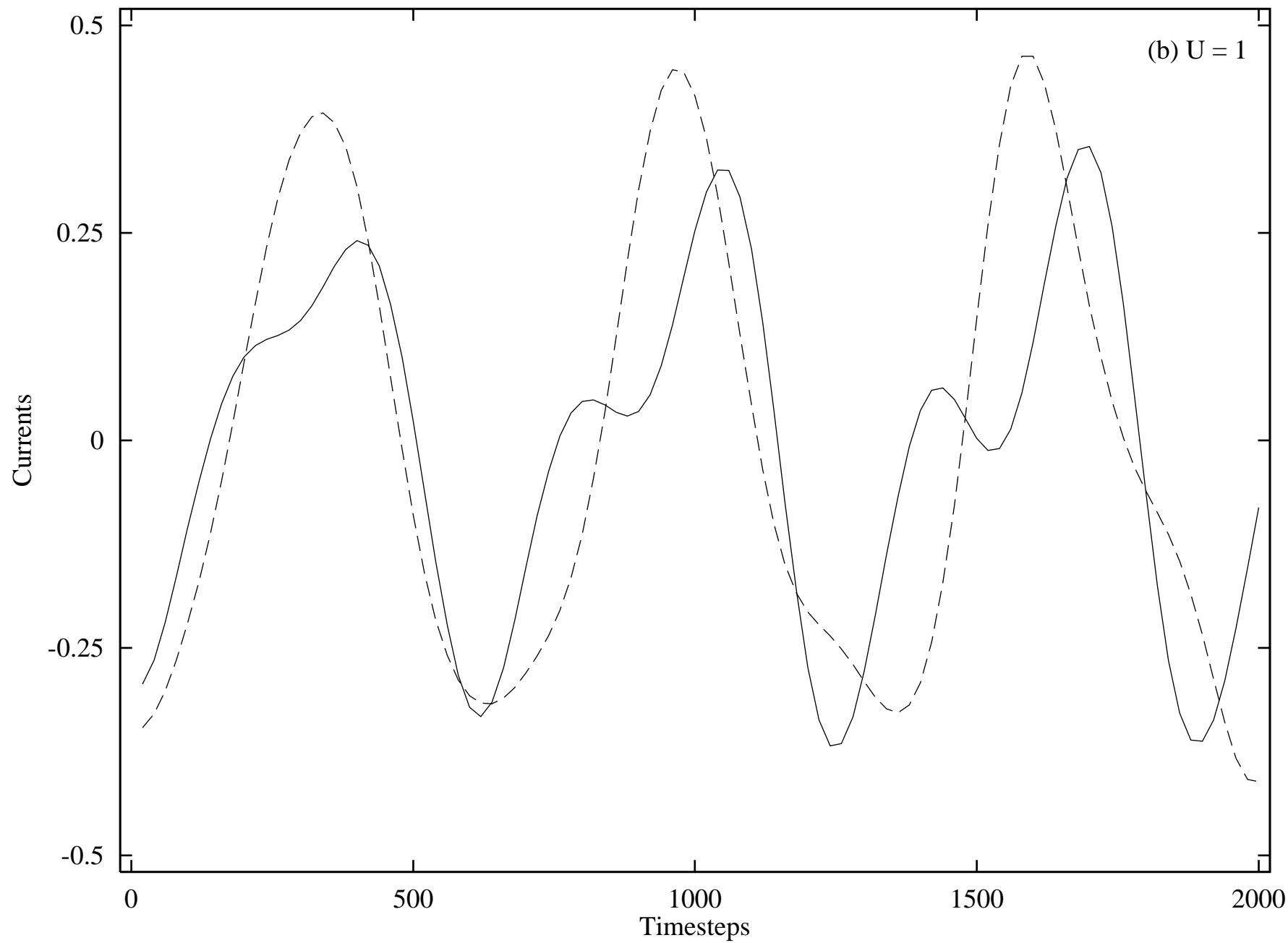


Fig. 1(c)

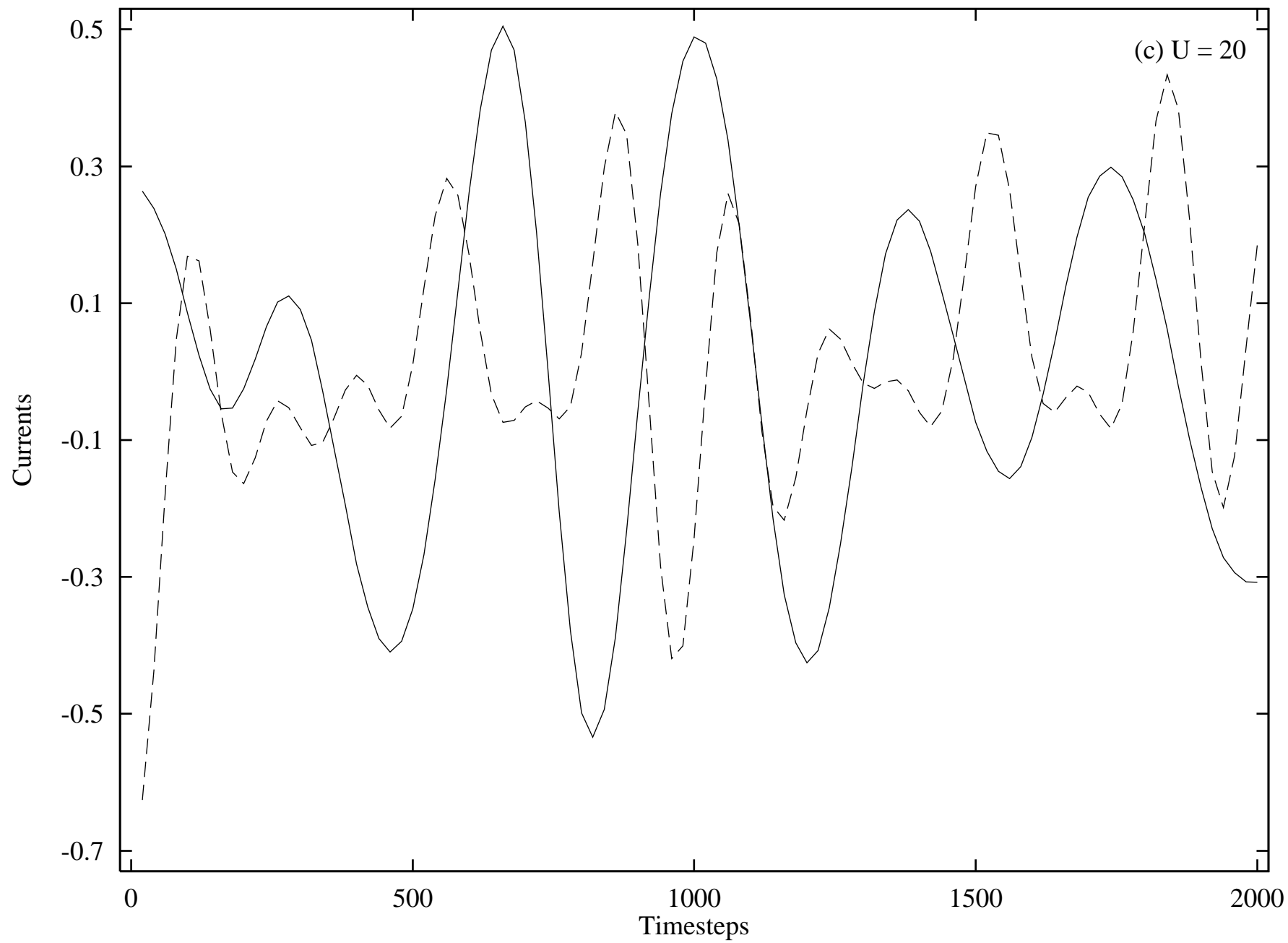


Fig. 2

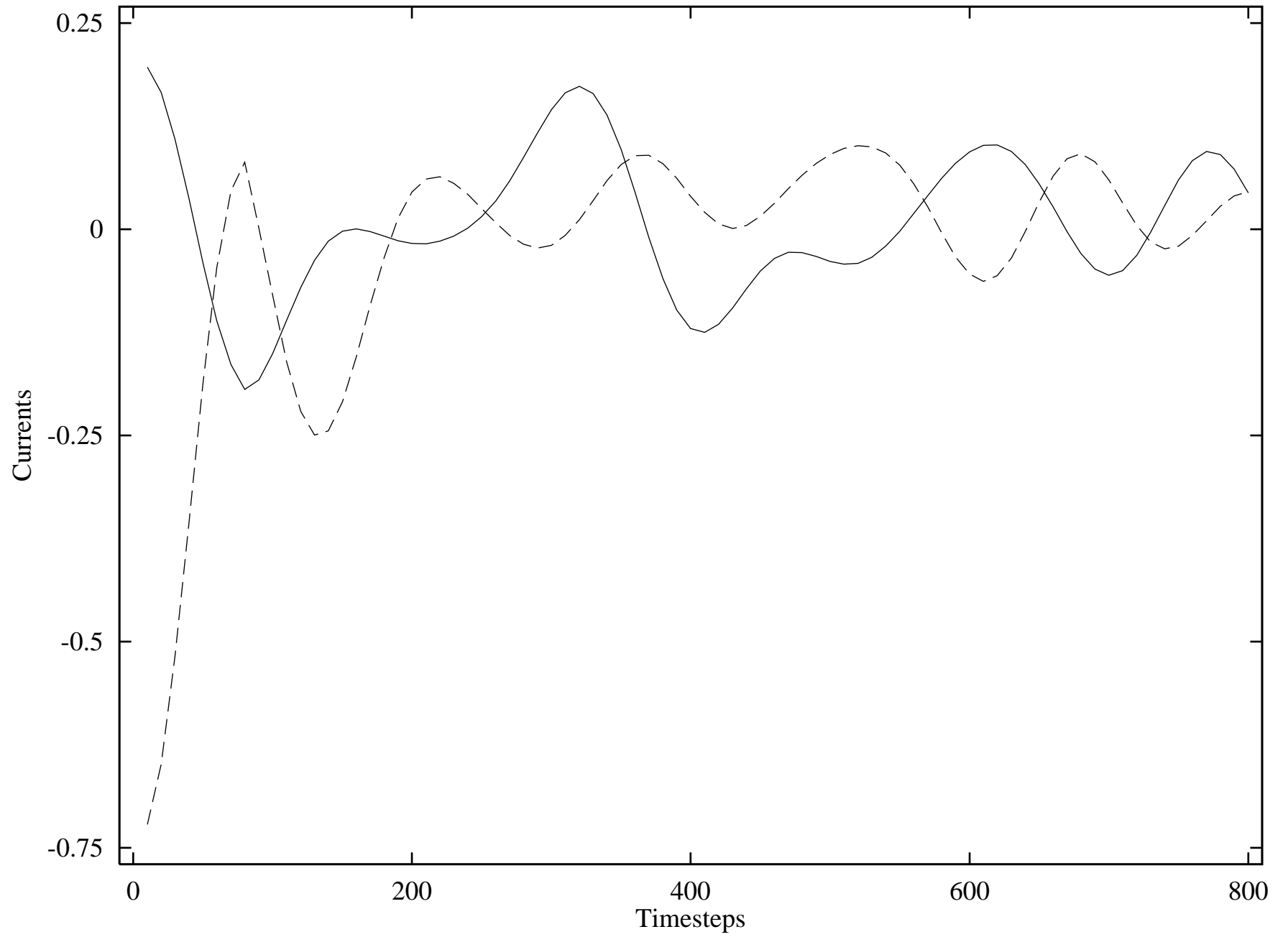


Fig. 3(a)

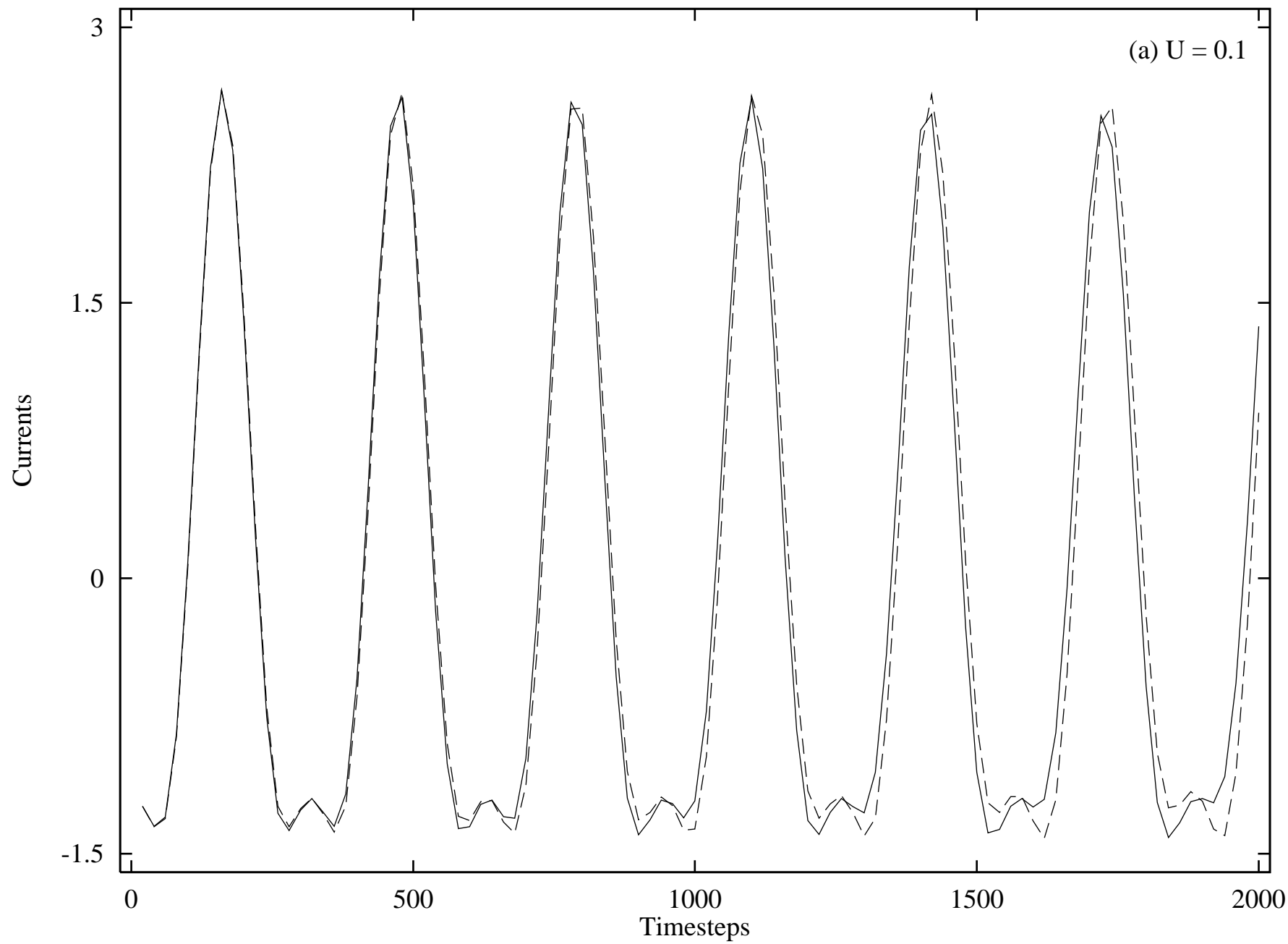


Fig. 3(b)

