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# Current density and continuity in discretized models

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## Abstract

Discrete approaches have long been used in numerical modelling of physical systems in both research and teaching. Discrete versions of the Schrödinger equation employing either one or several basis functions per mesh point are often used by senior undergraduates and beginning graduate students in computational physics projects. In studying discrete models, students can encounter conceptual difficulties with the representation of the current and its divergence because different finite-difference expressions, all of which reduce to the current density in the continuous limit, measure different physical quantities. Understanding these different discrete currents is essential and requires a careful analysis of the current operator, the divergence of the current and the continuity equation. Here we develop point forms of the current and its divergence valid for an arbitrary mesh and basis. We show that in discrete models currents exist only along lines joining atomic sites (or mesh points). Using these results, we derive a discrete analogue of the divergence theorem and demonstrate probability conservation in a purely localized-basis approach.

## 1. Introduction

Most interesting physical systems are governed by differential equations (e.g. the Schrödinger equation or Maxwell's equations) and, as well known, admit precious few analytic solutions. Numerical methods for solving these equations have therefore become a staple of both research and teaching in physics. Examples in our own field of nanoelectronics are the multi-band device simulators NEMO 1D [1], NEMO 3D [2] and OMEN [3]. These simulators employ a basis of localized atomic-like basis functions, having symmetry properties like the orbitals of atomic physics. Similar models, albeit with much smaller basis sets, have been used in

undergraduate or graduate courses [4–6]. The familiar finite-difference Schrödinger equation is in fact a special case of such a model, with one spherically symmetric basis function on each mesh point. Students often write programs to solve the finite-difference Schrödinger equation in their numerical methods and physics classes; they might also use more powerful approaches implemented as tools [8]. Senior undergraduates and graduate students therefore encounter discrete models generally and discrete versions of the Schrödinger equation especially in classes and research projects.

One difficulty students often encounter with discretized models is understanding the very different way in which the relevant physics is expressed in a discrete model versus its continuous antecedent. This difficulty can occur with the discrete approximation to any differential operator; however, it is best illustrated by concentrating on a specific system. Students of physics, chemistry and electrical engineering generally encounter the Schrödinger equation, so here we discuss problems in discretized quantum mechanics. As an example, we point to the treatment of the simplest quantum-mechanical problems, the infinite and finite square wells [4, 5]. For example, in the discretized infinite square well of nine sites the  $n = 1$  and  $n = 9$  wavefunctions appear identical, whereas in the continuous model they are clearly different. Another difference is that a magnetic vector potential is included via the Peierls-coupling method [9–11] in discrete models in order to maintain gauge invariance. Students can, however, come to understand these differences without undue effort since in both cases the relevant references thoroughly explain them and how they arise from discrete versions of continuous quantum mechanics.

In contrast to these relatively well-developed and explained aspects of discrete models, two important issues in discretized quantum mechanics, the representation of the current density and its divergence, are hardly ever discussed in texts and indeed are not nearly as well treated in the literature. In a finite-difference model the conceptual difficulty arises because there is no obvious choice for the representation of a derivative on a mesh. Forward-, backward- and central-difference formulae all reduce to the same point derivative in the limit of zero mesh spacing, yet each involves function values sampled on a different set of mesh points. Compounding the problem for the current and its divergence is the fact that the divergence, while a scalar, involves the second derivative of the wavefunction. The problem becomes all the more nettlesome when one is dealing with an expansion of the sampled function in a basis defined through its Hamiltonian matrix elements instead of explicit samples of the function (see section 2 below). Not surprisingly, these subtleties have led to a variety of expressions for the current and divergence [9, 12–15], some of which are correct but not fully explained [9, 14, 15], and others of which are incorrect [12, 13]. Several issues therefore require resolution, as discussed below.

First, a fully general, mesh- and basis-independent, treatment of the point form of the continuity equation has not been established to date. Second, while the difference between the continuous and discrete point current operators on a square mesh has been noted [14, 15], the origins of this difference and its implications for the discrete continuity equation remain unexplained. Explaining this distinction is necessary because in a discrete model, the entire concept of current density becomes problematic, and in any event different currents, all of which reduce to the continuous current density in the limit of zero mesh spacing, represent different physical quantities. Essentially the problem of the current density in a discrete model arises from the fact that in such a model the functions are sampled only on discrete points, so that bounding surfaces become somewhat fictitious, and a true discrete divergence theorem ought to involve only the sampled points. Finally, because the formalism should not require the mesh to be square, cubic or even regular, a general treatment of the discrete current and continuity equation is needed. Working strictly in a localized-orbital

basis, without assuming a regular mesh, we derive expressions for the current operator in both its point and total formulations, establish probability and current conservation and derive a discrete version of the divergence theorem. First we present general results for a basis set consisting of multiple functions per mesh point, then show how these reduce to the familiar finite-difference expressions. In so doing we explain why the current plays a different role in the discrete divergence theorem from that in the continuous case.

## 2. Model and discussion

Before examining how the discrete probability current, a vector function, differs from discrete scalar functions such as the probability density, it is helpful to discuss the process of discretization itself and the representations of functions on a mesh of finite spacing. Although most of our treatment is applicable to discretizing any linear differential system, we specialize to the Schrödinger equation and Hamiltonian operator in order to make the discussion more concrete and simple.

First, it should be recognized that the mesh need not be regular (e.g. cubic, square or triangular). Indeed, in molecular and condensed-matter physics the mesh points are usually dictated by the positions of the atoms in the molecule or crystal being modelled. Therefore in the development below, we use the terms ‘atom’ and ‘mesh point’ interchangeably. Thus a general mesh can have irregular distances and angles between points (atoms), and the formalism needs to accommodate this possibility.

Second, while the traditional treatment of the discrete Schrödinger equation is a strictly finite-difference approach, namely sampling the wavefunction on the mesh points, this is not the only way to solve the problem. One can, after all, expand the wavefunction in some basis most conveniently one consisting of a set of localized functions centred on each mesh point or atom:  $\varphi_\gamma(\mathbf{r} - \mathbf{R}_m) = \langle \mathbf{r} | \gamma; \mathbf{R}_m \rangle$ , where  $\gamma$  is the function index (we assume the same set is used on each atom) and  $\mathbf{R}_m$  is the location of the atom. As is customary, the basis is assumed orthonormal,  $\langle \eta; \mathbf{R}_l | \gamma; \mathbf{R}_m \rangle = \delta_{\gamma,\eta} \delta_{l,m}$ , and Hamiltonian matrix elements between basis functions on atoms (mesh points) separated beyond a cutoff distance are assumed to vanish. (In molecular and condensed-matter physics this type of model is referred to as a ‘tight-binding’ model, especially when the basis functions are atomic-like.) Quite often the basis is defined implicitly, through its Hamiltonian matrix elements, as opposed to explicit real-space representations of the functions. We consider this case here, and in this treatment solving the discrete Schrödinger equation yields the expansion coefficients (indexed by basis function and atom) instead of a direct sampling of the wavefunction itself. This multi-component approach is often more accurate than simply sampling the wavefunction and recalls the method of interpolating functions from numerical analysis.

As one might expect, the traditional finite-difference treatment of the Schrödinger equation is a single-component special case of the multi-component approach. In fact, the finite-difference (3D) Schrödinger equation results when one takes a cubic mesh and a basis of one spherically symmetric function per mesh point, with the only non-zero Hamiltonian matrix elements being between basis functions on the same or nearest-neighbour mesh points (atoms). The expansion coefficients in this case are samples of the wavefunction on the mesh points. Having set out some general considerations regarding discretization, we derive expressions for the current and its divergence in terms of the expansion coefficients, Hamiltonian matrix elements and atomic positions for both the multiple- and single-component bases. We then connect the current and its divergence in discrete forms of the divergence theorem and continuity equation.

### 2.1. Discretized current: general multi-component model

It is most convenient to begin with the particle current in the localized-orbital basis. In analogy with continuous quantum mechanics, we define point ( $\hat{j}_m^{(\mu)}$ ) and total ( $\hat{J}^{(\mu)}$ ) particle current operators along a direction specified by the unit vector  $\mathbf{e}_\mu$  as

$$\hat{j}_m^{(\mu)} = \frac{1}{2} \{ \hat{n}_m \hat{v}^{(\mu)} + \hat{v}^{(\mu)} \hat{n}_m \}; \quad \hat{J}^{(\mu)} = \sum_m \hat{j}_m^{(\mu)}, \quad (1)$$

where  $m$  indexes atoms, located at positions  $\mathbf{R}_m$ . In Cartesian coordinates  $\mathbf{R}_m$  is written as  $\mathbf{R}_m = R_m^{(x)} \mathbf{e}_x + R_m^{(y)} \mathbf{e}_y + R_m^{(z)} \mathbf{e}_z$ ; we denote the component of  $\mathbf{R}_m$  along an arbitrary direction  $\mathbf{e}_\mu$  (not necessarily one of the Cartesian axes) by  $R_m^{(\mu)}$ . In equation (1) the velocity operator is

$$\hat{v}^{(\mu)} = \frac{1}{i\hbar} [\hat{r}^{(\mu)}, \hat{H}], \quad (2)$$

while the point density operator for the atom at  $\mathbf{R}_m$  is

$$\hat{n}_m = \sum_\gamma |\gamma; \mathbf{R}_m\rangle \langle \gamma; \mathbf{R}_m|, \quad (3)$$

where  $|\gamma; \mathbf{R}_m\rangle$  is the basis function of type or index  $\gamma$  centred on the atom at  $\mathbf{R}_m$ . We take the position operator to be strictly diagonal in order to guarantee gauge invariance [9–11, 16] in an arbitrary basis:

$$\langle \alpha'; \mathbf{R}_{n'} | \hat{r}^{(\mu)} | \alpha; \mathbf{R}_n \rangle = R_n^{(\mu)} \delta_{\alpha', \alpha} \delta_{n', n}, \quad (4)$$

so that the velocity matrix elements are

$$\langle \alpha'; \mathbf{R}_{n'} | \hat{v}^{(\mu)} | \alpha; \mathbf{R}_n \rangle = \frac{1}{i\hbar} (R_{n'}^{(\mu)} - R_n^{(\mu)}) \langle \alpha'; \mathbf{R}_{n'} | \hat{H} | \alpha; \mathbf{R}_n \rangle. \quad (5)$$

Note that in the presence of electromagnetic fields the Hamiltonian matrix element in equation (5) is computed using the Peierls-coupling method [9–11].

Comparing the expectation values of the point and total current operators is revealing. For an arbitrary state  $|\psi\rangle$ , one has

$$|\psi\rangle = \sum_l |\psi_l\rangle; \quad |\psi_l\rangle = \sum_\eta c_{\eta,l}(t) |\eta; \mathbf{R}_l\rangle. \quad (6)$$

Note that the expansion coefficients  $c_{\eta,l}(t)$  might depend on time. Equations (1)–(6) give

$$\langle \psi | \hat{j}_m^{(\mu)} | \psi \rangle = \sum_l j_{(l,m)}^{(\mu)}; \quad \langle \psi | \hat{J}^{(\mu)} | \psi \rangle = \sum_{l,m} j_{(l,m)}^{(\mu)}, \quad (7)$$

where the partial current along the straight-line path from  $\mathbf{R}_m$  to  $\mathbf{R}_l$  is

$$j_{(l,m)}^{(\mu)} = \frac{1}{i2\hbar} (R_l^{(\mu)} - R_m^{(\mu)}) \sum_{\gamma,\eta} \{ c_{\gamma,m} c_{\eta,l}^* \langle \eta; \mathbf{R}_l | \hat{H} | \gamma; \mathbf{R}_m \rangle - c_{\eta,l} c_{\gamma,m}^* \langle \gamma; \mathbf{R}_m | \hat{H} | \eta; \mathbf{R}_l \rangle \}. \quad (8)$$

In equation (8) we suppress the possible time dependence of the expansion coefficients for brevity.

Two remarkable facts stand out on examination of equations (6)–(8). First, it is clear that currents are only defined along straight-line paths between atoms, which we shall call ‘links’, with no same-atom contribution to the current. Therefore currents cannot be probed off of these paths, just as the probability density cannot be probed off of atomic sites. Thus the current density is not a continuous function over a surface. As a corollary, the entire concept of a bounding surface becomes somewhat arbitrary and problematic, so care must be taken in deriving the discrete divergence theorem. Second, comparing equations (7) and (8) shows

that the total current along the straight-line path ( $\mathbf{R}_l - \mathbf{R}_m$ ) is composed of two contributions,  $j_{(l,m)}^{(\mu)}$  and  $j_{(m,l)}^{(\mu)}$ . These two contributions are exactly equal since

$$j_{(m,l)}^{(\mu)} = \frac{1}{i2\hbar} (R_m^{(\mu)} - R_l^{(\mu)}) \sum_{\alpha,\beta} \{c_{\alpha,l} c_{\beta,m}^* \langle \beta; \mathbf{R}_m | \hat{H} | \alpha; \mathbf{R}_l \rangle - c_{\beta,m} c_{\alpha,l}^* \langle \alpha; \mathbf{R}_l | \hat{H} | \beta; \mathbf{R}_m \rangle\} = j_{(l,m)}^{(\mu)}, \quad (9)$$

where the last equality follows on multiplying both the prefactor and sum by  $-1$  and renaming  $(\alpha, \beta) = (\eta, \gamma)$ , as they are merely dummy indices of summation. Using equations (8) and (9) the total current in the link ( $\mathbf{R}_l - \mathbf{R}_m$ ), defined as  $\mathbf{J}_{(l,m)}$ , is easily found:

$$\mathbf{J}_{(l,m)} = \mathbf{j}_{(l,m)} + \mathbf{j}_{(m,l)} = \frac{(\mathbf{R}_l - \mathbf{R}_m)}{i\hbar} \sum_{\gamma,\eta} \{c_{\gamma,m} c_{\eta,l}^* \langle \eta; \mathbf{R}_l | \hat{H} | \gamma; \mathbf{R}_m \rangle - c_{\eta,l} c_{\gamma,m}^* \langle \gamma; \mathbf{R}_m | \hat{H} | \eta; \mathbf{R}_l \rangle\} \quad (10)$$

$$\mathbf{J}_{(l,m)} = \frac{1}{i\hbar} |\mathbf{R}_l - \mathbf{R}_m| [\langle \psi_l | \hat{H} | \psi_m \rangle - \langle \psi_m | \hat{H} | \psi_l \rangle] \mathbf{e}_{(l,m)}; \quad \mathbf{e}_{(l,m)} = \frac{\mathbf{R}_l - \mathbf{R}_m}{|\mathbf{R}_l - \mathbf{R}_m|}, \quad (11)$$

where equation (6) was used to rewrite equation (11) from equation (10). Note that equation (11) shows explicitly that both the prefactor  $(\mathbf{R}_l - \mathbf{R}_m)$  and sum in equation (10) vanish for  $l = m$ , and that there are no same-atom contributions to the current nor to the sum in equation (10).

## 2.2. Discretized current: finite-difference Schrödinger equation

The preceding general multi-component expressions might not seem familiar on first examination, and the conclusion that only currents along links (as opposed to current densities) can be represented might likewise seem peculiar, yet both the form taken by the current and the physical significance of the link currents follow directly from the finite-difference Schrödinger equation. These parallels are not accidental, since the mathematical structure of a multi-component model is identical to that of finite-difference equations for a vector-valued function. As discussed in [4, 5, 7] the finite-difference (effective-mass) Schrödinger equation is identical to a model having only one spherically symmetric basis function per point, deployed on a cubic mesh of spacing,  $a$ .

Because the mesh is regular and there is only one orbital type per atom (mesh point), the notation is considerably simplified by dropping the orbital-type designation and indexing the atoms by the ordered triples,  $(l, m, n)$ , where the atomic positions are given by  $\mathbf{R}_{l,m,n} = a(l\mathbf{e}_x + m\mathbf{e}_y + n\mathbf{e}_z)$ . From [7] the matrix elements of the Hamiltonian in a single material with effective mass,  $m_e$ , and including an applied potential,  $U$ , are

$$\begin{aligned} \langle l, m, n | \hat{H} | l', m', n' \rangle &= \left( \frac{6\hbar^2}{2m_e a^2} + U_{l,m,n} \right) \delta_{l,l'} \delta_{m,m'} \delta_{n,n'} - \frac{\hbar^2}{2m_e a^2} \\ &\times (\delta_{l\pm 1, l'} \delta_{m,m'} \delta_{n,n'} + \delta_{l,l'} \delta_{m\pm 1, m'} \delta_{n,n'} + \delta_{l,l'} \delta_{m,m'} \delta_{n\pm 1, n'}), \end{aligned} \quad (12)$$

where the wavefunction is written as

$$|\psi\rangle = \sum_{l', m', n'} \psi_{l', m', n'} |l', m', n'\rangle, \quad (13)$$

with  $|l, m, n\rangle$  denoting the (spherically symmetric) basis function at atom (mesh point)  $\mathbf{R}_{l,m,n}$ . The expansion coefficients  $\psi_{l,m,n}$  are samples of the continuous wavefunction on the mesh points:  $\psi_{l,m,n} = \psi(\mathbf{R}_{l,m,n})$ .

From the symmetry of the mesh it suffices to consider only one component of the current; for convenience we choose the  $x$ -component. Substituting matrix elements (12) and wavefunction (13) into equation (9) yields the partial link currents to the neighbouring atoms (mesh points). A straightforward calculation shows that the only non-vanishing partial link currents are those from  $(l, m, n)$  to  $(l \pm 1, m, n)$ :

$$j_{(l,m,n),(l\pm 1,m,n)}^{(x)} = \pm \frac{\hbar}{i2m_e} \frac{1}{2a} \{ \psi_{l,m,n}^* \psi_{l\pm 1,m,n} - \psi_{l\pm 1,m,n}^* \psi_{l,m,n} \}. \quad (14)$$

As discussed in the previous section, the total link currents are twice the partial link currents,  $J_{(l,m,n),(l\pm 1,m,n)}^{(x)} = 2j_{(l,m,n),(l\pm 1,m,n)}^{(x)}$ . From equation (7), the  $x$ -component of the point current is simply

$$\begin{aligned} j_{(l,m,n)}^{(x)} &= j_{(l,m,n),(l+1,m,n)}^{(x)} + j_{(l,m,n),(l-1,m,n)}^{(x)} \\ &= \frac{\hbar}{i2m_e} \left\{ \psi_{l,m,n}^* \frac{(\psi_{l+1,m,n} - \psi_{l-1,m,n})}{2a} - \psi_{l,m,n} \frac{(\psi_{l+1,m,n}^* - \psi_{l-1,m,n}^*)}{2a} \right\}, \end{aligned} \quad (15)$$

while the three currents  $J_{(l,m,n),(l\pm 1,m,n)}^{(x)}$  and  $j_{(l,m,n)}^{(x)}$  clearly represent different quantities in the discrete model, each is in fact a finite-difference approximation for the continuous current  $j^{(x)}(\mathbf{R}_{l,m,n})$ . This limit is obvious in the case of the point current, equation (15), using the central difference approximation

$$\frac{\psi_{l+1,m,n} - \psi_{l-1,m,n}}{2a} \approx \frac{\partial \psi}{\partial x}(\mathbf{R}_{l,m,n}) \quad (16)$$

so one finds

$$\lim_{a \rightarrow 0} j_{(l,m,n)}^{(x)} = \frac{\hbar}{i2m_e} \left\{ \psi^*(\mathbf{R}_{l,m,n}) \frac{\partial \psi}{\partial x}(\mathbf{R}_{l,m,n}) - \psi(\mathbf{R}_{l,m,n}) \frac{\partial \psi^*}{\partial x}(\mathbf{R}_{l,m,n}) \right\}. \quad (17)$$

For the link currents  $J_{(l,m,n),(l\pm 1,m,n)}^{(x)}$  this limit is demonstrated using the forward- and backward-difference formulae

$$\frac{\psi_{l+1,m,n} - \psi_{l,m,n}}{a} \approx \frac{\partial \psi}{\partial x}(\mathbf{R}_{l,m,n}), \quad \frac{\psi_{l,m,n} - \psi_{l-1,m,n}}{a} \approx \frac{\partial \psi}{\partial x}(\mathbf{R}_{l,m,n}) \quad (18)$$

in equation (14) to find

$$\begin{aligned} \lim_{a \rightarrow 0} J_{(l,m,n),(l\pm 1,m,n)}^{(x)} &= 2 \lim_{a \rightarrow 0} j_{(l,m,n),(l\pm 1,m,n)}^{(x)} \\ &= \frac{\hbar}{i2m_e} \left\{ \psi^*(\mathbf{R}_{l,m,n}) \frac{\partial \psi}{\partial x}(\mathbf{R}_{l,m,n}) - \psi(\mathbf{R}_{l,m,n}) \frac{\partial \psi^*}{\partial x}(\mathbf{R}_{l,m,n}) \right\}. \end{aligned} \quad (19)$$

An additional property common to all three of these currents as well as those in a general multi-component model (discussed above) is that currents only exist along links (here lines between mesh points). Nevertheless, in a discrete sense these three currents measure different physical quantities. The link currents  $J_{(l,m,n),(l\pm 1,m,n)}^{(x)}$  measure the total current in the links  $(l, m, n) \leftrightarrow (l \pm 1, m, n)$ , while the point current  $j_{(l,m,n)}^{(x)}$  consists of two partial link currents, but to *different* links: one each to  $(l \pm 1, m, n)$ . The distinction is not academic: computers can only deal with discrete equations and the fact that all three currents have the same limit is in some sense irrelevant as setting  $a = 0$  invites a core dump. Moreover there remains the important question of which current, the link current or the point current, is the more physically relevant for continuity. The answer lies in the discrete approximation for the divergence of the current.

### 2.3. Discretized divergence: general multi-component and finite-difference

We next consider the divergence of the current, which may be derived in several different ways. In continuous quantum mechanics, one has

$$\nabla \cdot \hat{\mathbf{J}}(\mathbf{r}, \mathbf{r}') = -\frac{1}{i\hbar} [\delta^3(\mathbf{r} - \mathbf{r}'), \hat{H}(\mathbf{r}')], \quad (20)$$

so that its discrete analogue is

$$\nabla \cdot \hat{\mathbf{J}}_m = -\frac{1}{i\hbar} [\hat{n}_m, \hat{H}], \quad J_m^{(\mu)} = \sum_l J_{(l,m)}^{(\mu)}, \quad (21)$$

where  $J_m^{(\mu)}$  is the total link current along  $\mathbf{e}_\mu$  for the  $m$ th atom. As we show below in connection with probability conservation, it is the total link current for the  $m$ th atom which must appear in the discrete expression, equation (21), unlike in continuous quantum mechanics, equation (20), where the point current, whose discrete analogue is equation (1), appears. Certainly the discrete result makes physical sense since it is the link currents which determine the rate of change of probability density at an atom. Using equations (6) and (21)

$$\langle \psi | \nabla \cdot \hat{\mathbf{J}}_m | \psi \rangle = \frac{1}{i\hbar} \sum_l \sum_{\gamma, \eta} \{c_{\gamma,m} c_{\eta,l}^* \langle \eta; \mathbf{R}_l | \hat{H} | \gamma; \mathbf{R}_m \rangle - c_{\eta,l} c_{\gamma,m}^* \langle \gamma; \mathbf{R}_m | \hat{H} | \eta; \mathbf{R}_l \rangle\}. \quad (22)$$

We remark that equation (22) is also consistent with a finite-difference approximation. Because currents are only defined along links, the discrete divergence reduces to a single discrete derivative, namely that with respect to  $r_{(l,m)} = |\mathbf{R}_l - \mathbf{R}_m|$  of the current  $\mathbf{J}_{(l,m)}$ . With  $\mathbf{J}_{(l,m)} = J_{(l,m)}(\mathbf{r}_{(l,m)})\mathbf{e}_{(l,m)}$ , the forward difference formula gives

$$[\nabla \cdot \mathbf{J}]_{(l,m)} \approx \frac{J_{(l,m)}(r_{(l,m)}) - J_{(l,m)}(0)}{r_{(l,m)}} = \frac{1}{i\hbar} [\langle \psi_l | \hat{H} | \psi_m \rangle - \langle \psi_m | \hat{H} | \psi_l \rangle]. \quad (23)$$

Summing over all partial divergences for the atom at  $\mathbf{R}_m$  once again gives equation (22):

$$\langle \psi | \nabla \cdot \hat{\mathbf{J}}_m | \psi \rangle = \sum_l [\nabla \cdot \mathbf{J}]_{(l,m)} = \frac{1}{i\hbar} \sum_l [\langle \psi_l | \hat{H} | \psi_m \rangle - \langle \psi_m | \hat{H} | \psi_l \rangle]. \quad (24)$$

The counterpart of equations (8) or (22) in the finite-difference Schrödinger equation on a square mesh is discussed in Baranger *et al* [14, 15]; they additionally observe that the point current operator does not measure the current in a link between mesh points but do not discuss the reasons for the difference. For the finite-difference Schrödinger equation on a cubic grid as discussed in section 2.2 above, the discrete divergence is simply

$$\begin{aligned} \langle \psi | \nabla \cdot \hat{\mathbf{J}}_{(l,m,n)} | \psi \rangle &= \frac{1}{i\hbar} \sum_{l',m',n'} \{ \psi_{l,m,n} \psi_{l',m',n'}^* \langle l', m', n' | \hat{H} | l, m, n \rangle \\ &\quad - \psi_{l',m',n'} \psi_{l,m,n}^* \langle l, m, n | \hat{H} | l', m', n' \rangle \}. \end{aligned} \quad (25)$$

Using equation (12) for the Hamiltonian matrix elements and the familiar central difference approximations for the second derivatives,

$$\frac{\partial^2 \psi}{\partial x^2}(\mathbf{R}_{l,m,n}) \approx \frac{1}{a^2} [\psi_{l+1,m,n} - 2\psi_{l,m,n} + \psi_{l-1,m,n}], \quad \text{etc}, \quad (26)$$

it follows that the divergence has the expected limit as  $a \rightarrow 0$ :

$$\lim_{a \rightarrow 0} \langle \psi | \nabla \cdot \hat{\mathbf{J}}_{(l,m,n)} | \psi \rangle = \frac{\hbar}{i2m_e} \{ \psi^*(\mathbf{R}_{l,m,n}) \nabla^2 \psi(\mathbf{R}_{l,m,n}) - \psi(\mathbf{R}_{l,m,n}) \nabla^2 \psi^*(\mathbf{R}_{l,m,n}) \}. \quad (27)$$

#### 2.4. Current continuity

From the discussion in sections 2.2 and 2.3 above it is apparent that in a discrete model (either single- or multi-component), the concept of current density is no longer useful. Instead one has discrete currents along lines connecting mesh points (atoms). The structure of discrete models is therefore much more like that of classical lumped-parameter circuits, where only total currents (as opposed to current densities) are relevant and bounding surfaces are rather arbitrary. We therefore expect the continuity equation to take a different form, appearing *in structure* more like Kirchoff's current law of classical circuits, except that in this case charge *can* accumulate at a node (i.e. mesh point or atom). A natural place to begin the investigation of current continuity is with the finite-difference Schrödinger equation.

In this model, a more illuminating expression for the divergence of the current than that in equation (27) can be derived by returning to equation (25) and observing that all terms in  $|\psi_{l,m,n}|^2$  cancel so that

$$\langle \psi | \nabla \cdot \hat{\mathbf{J}}_{(l,m,n)} | \psi \rangle = \frac{\hbar}{i2m_e a^2} \{ \psi_{l,m,n}^* [\psi_{l+1,m,n} + \psi_{l-1,m,n}] - \psi_{l,m,n} [\psi_{l+1,m,n}^* + \psi_{l-1,m,n}^*] + \text{c.p.} \}. \quad (28)$$

In equation (28) c.p. denotes cyclic permutations, i.e. terms in  $(l, m \pm 1, n)$  and  $(l, m, n \pm 1)$ . Equation (28) reveals a deep physical significance when we recognize that it can be expressed in terms of the currents along each link,

$$\begin{aligned} & \frac{\hbar}{i2m_e a^2} \{ \psi_{l,m,n}^* [\psi_{l+1,m,n} + \psi_{l-1,m,n}] - \psi_{l,m,n} [\psi_{l+1,m,n}^* + \psi_{l-1,m,n}^*] \} \\ &= \frac{1}{a} [\mathbf{J}_{(l,m,n),(l+1,m,n)} \cdot \mathbf{e}_{(l,m,n),(l+1,m,n)} + \mathbf{J}_{(l,m,n),(l-1,m,n)} \cdot \mathbf{e}_{(l,m,n),(l-1,m,n)}], \quad (29) \end{aligned}$$

with analogous expressions for the other two pairs of links, to  $(l, m \pm 1, n)$  and  $(l, m, n \pm 1)$ . In equation (29) the outward normals along the links are

$$\mathbf{e}_{(l,m,n),(l \pm 1,m,n)} = \pm \mathbf{e}_x, \quad \mathbf{e}_{(l,m,n),(l,m,\pm 1n)} = \pm \mathbf{e}_y, \quad \mathbf{e}_{(l,m,n),(l,m,n \pm 1)} = \pm \mathbf{e}_z. \quad (30)$$

Using equation (29) and its counterparts, equation (28) becomes a form of Gauss' divergence theorem,

$$a \langle \psi | \nabla \cdot \hat{\mathbf{J}}_{(l,m,n)} | \psi \rangle = \sum_{\substack{l',m',n' \\ \text{6 NN links}}} \mathbf{J}_{(l,m,n),(l',m',n')} \cdot \mathbf{e}_{(l,m,n),(l',m',n')}, \quad (31)$$

where the sum in equation (31) is over the six nearest-neighbour links,  $(l', m', n') = \{(l \pm 1, m, n), (l, m \pm 1, n), (l, m, n \pm 1)\}$ . Equation (31) shows that the link current, and not the point current, is the more physically relevant for continuity in the finite-difference Schrödinger equation. The fact that this model is mathematically a special case of multi-component models strongly suggests that in a general discrete model the link currents should likewise be the physically relevant quantities.

In fact, the reason for the significance of the link current in either model arises from the geometry of the discretization process itself. When discretizing a scalar field  $f(\mathbf{r})$  on a uniform grid, it takes *two* samples to approximate each derivative  $\partial f / \partial r^{(\mu)}$ . Because each point on the grid must be treated on an equal footing, one-half of the derivative is associated with each of the sample points. Hence the point current includes only one-half of each link current.

The detailed reason why the point and link currents measure different observables, as well as which is relevant for charge conservation, can be determined by deriving a version of Gauss' divergence theorem relating the Laplacian,  $\nabla^2 f = \nabla \cdot (\nabla f)$ , and gradient,  $\nabla f$ , of a scalar

field  $f(\mathbf{r})$ . Consider a box of volume  $\Delta x \Delta y \Delta z$  centred at the point  $\mathbf{r}_0 = (r_0^{(x)}, r_0^{(y)}, r_0^{(z)})$ , and at the centre of each face,  $\mathbf{r}_F$ , compute dot products of  $\nabla f$  with the respective outward normal,  $\mathbf{e}_F$ :

$$\sum_{\text{faces}, i} [\nabla f \cdot \mathbf{e}_{F,i}]_{\mathbf{r}_{F,i}} = \sum_{\mu=\{x,y,z\}} \left\{ \frac{\partial f}{\partial r^{(\mu)}} \left( \mathbf{r}_0 + \frac{\Delta\mu}{2} \mathbf{e}_\mu \right) - \frac{\partial f}{\partial r^{(\mu)}} \left( \mathbf{r}_0 - \frac{\Delta\mu}{2} \mathbf{e}_\mu \right) \right\} \quad (32)$$

$$\sum_{\text{faces}, i} [\nabla f \cdot \mathbf{e}_{F,i}]_{\mathbf{r}_{F,i}} \approx \sum_{\mu=\{x,y,z\}} \Delta\mu \left\{ \left[ \frac{f(\mathbf{r}_0 + \Delta\mu \mathbf{e}_\mu) - f(\mathbf{r}_0)}{(\Delta\mu)^2} \right] - \left[ \frac{f(\mathbf{r}_0) - f(\mathbf{r}_0 - \Delta\mu \mathbf{e}_\mu)}{(\Delta\mu)^2} \right] \right\} \quad (33)$$

$$\sum_{\text{faces}, i} [\nabla f \cdot \mathbf{e}_{F,i}]_{\mathbf{r}_{F,i}} \approx \sum_{\mu=\{x,y,z\}} (\Delta\mu) \frac{\partial^2 f}{\partial r^{(\mu)2}}(\mathbf{r}_0). \quad (34)$$

Equation (34) is clearly a discrete form of Gauss' divergence theorem, with the discrete (closed) surface integral appearing on the left and the discrete volume integral on the right; note that equation (31) is also in this form. If we take a grid with spacing  $\Delta\mu$  along the  $\mathbf{e}_\mu$ ,  $\mu \in \{x, y, z\}$  axis, equation (33) shows that it is the 'link gradient' (analogue of the link current) for each face which appears in the discrete divergence theorem, not the point gradient. That is, the link gradient samples  $\nabla f$  at the midpoint between the two grid points in a link, and it is the sum of these link gradients which is related to the point divergence.

This discrete version of Gauss' divergence theorem is easily modified in the multi-component treatment, allowing us to show that equations (11) and (23) also satisfy a discrete divergence theorem. Of course, in a general discrete model the mesh points might be fixed by actual atomic positions, so it is impossible to evaluate the current at the midpoint of a link, yet the interpretation of equation (34) is a reasonable one. We proceed from equation (33) because it involves only samples of the scalar field evaluated at the grid points, avoiding problems associated with calculating gradients in an arbitrary discrete model: even where one has an explicit wavefunction calculating the divergence of the current at an arbitrary point will require the explicit relationship between the momentum operator and spatial differentiation for the particular model used. (They cannot be the same operator in any finite-dimension basis, as shown by Graf and Vogl [9]. Note that even in the linear augmented plane wave method a special  $\mathbf{k} \cdot \mathbf{p}$  formula is necessary [17].) In the sum on the right-hand side of equation (33) we recognize each term in square brackets as a partial divergence, while the prefactor  $\Delta\mu$  is the associated link length. Thus the general discrete analogue is

$$|\mathbf{R}_l - \mathbf{R}_m| [\nabla \cdot \mathbf{J}]_{(l,m)} = \frac{1}{i\hbar} |\mathbf{R}_l - \mathbf{R}_m| [\langle \psi_l | \hat{H} | \psi_m \rangle - \langle \psi_m | \hat{H} | \psi_l \rangle]. \quad (35)$$

Note that in general the link lengths and angles can differ, unlike in equations (32)–(34) where the links along a common axis are of the same length. On the left-hand side, it is clear that the dot products of the link currents and their associated outward normals appear. The analogous general discrete expression reads

$$\mathbf{J}_{(l,m)} \cdot \mathbf{e}_{(l,m)} = \frac{1}{i\hbar} |\mathbf{R}_l - \mathbf{R}_m| [\langle \psi_l | \hat{H} | \psi_m \rangle - \langle \psi_m | \hat{H} | \psi_l \rangle] = |\mathbf{R}_l - \mathbf{R}_m| [\nabla \cdot \mathbf{J}]_{(l,m)}. \quad (36)$$

Summing over links to neighbouring atoms,  $l$ , and taking advantage of the last equality in equation (36) give the discrete divergence theorem for the atom,  $m$ :

$$\sum_l \mathbf{J}_{(l,m)} \cdot \mathbf{e}_{(l,m)} = \sum_l |\mathbf{R}_l - \mathbf{R}_m| [\nabla \cdot \mathbf{J}]_{(l,m)}. \quad (37)$$

Observe that as equation (37) is satisfied for any atom,  $m$ , and neighbours,  $l$ , it holds for multi-atom volumes as well. (Recall that  $\mathbf{e}_{(m,l)} = -\mathbf{e}_{(l,m)}$  and  $[\nabla \cdot \mathbf{J}]_{(m,l)} = -[\nabla \cdot \mathbf{J}]_{(l,m)}$ .)

We remark that this derivation is fully consistent with the view that the currents calculated above are in fact filamentary currents and not current densities. We do not divide the current by a constant volume per atom to obtain a current density as do Graf and Vogl [9] in their treatment for periodic systems since we need a formalism valid in the more general non-periodic case, where defining a constant volume per atom may not be possible. Furthermore, the filamentary nature of the current makes defining bounding surfaces and enclosing volumes problematic, especially in the general, non-periodic case. Additionally, note that the number and arrangement of the mesh points might be completely determined by the atomic positions. This situation is different from even the finite-difference Schrödinger equation where both the grid spacing and geometry may be arbitrarily chosen to achieve the desired accuracy. In view of these difficulties, approaching the total current as a sum of one-dimensional currents seems the only consistent procedure.

Finally, we establish current continuity. We employ the point density operator, equation (3), although one could just as easily employ the density matrix for a pure state. Equations (3) and (6) give the probability density for the atom,  $m$ :

$$\langle \psi | \hat{n}_m | \psi \rangle = \sum_{\gamma} |c_{\gamma,m}|^2 = \rho_m. \quad (38)$$

Because  $\hat{n}_m$  has no explicit time dependence, Ehrenfest's theorem gives

$$\frac{d\rho_m}{dt} = -\frac{1}{i\hbar} \langle \psi | [\hat{H}, \hat{n}_m] | \psi \rangle \quad (39)$$

$$\begin{aligned} \frac{d\rho_m}{dt} &= -\frac{1}{i\hbar} \sum_l \sum_{\gamma,\eta} \{c_{\gamma,m} c_{\eta,l}^* \langle \eta; \mathbf{R}_l | \hat{H} | \gamma; \mathbf{R}_m \rangle - c_{\eta,l} c_{\gamma,m}^* \langle \gamma; \mathbf{R}_m | \hat{H} | \eta; \mathbf{R}_l \rangle\} \\ &= -\langle \psi | \nabla \cdot \mathbf{J}_m | \psi \rangle, \end{aligned} \quad (40)$$

where the last step in equation (39) follows from equation (21). Equations (21) and (39) or alternatively equations (22) and (40) establish probability conservation in point form. We reiterate the important point that the discretization process itself causes the link currents (as opposed to the point currents) to appear in the continuity equation. This situation is different from continuous quantum mechanics where there is only a point current, as there are no links. The discretized Schrödinger equation illustrates the conceptual difficulty: both the link currents and point currents become the point current in the limit of the grid spacing  $a \rightarrow 0$ , so without a careful analysis it is initially unclear which is the more physically meaningful one.

### 3. Conclusions

We have studied probability currents in single- and multi-component discrete models in detail, finding that currents are only defined along links (straight-line paths between atoms or mesh points) and that each of the atoms constituting the endpoints of a link accounts for one-half of the total current in the link. We have shown that the discrete divergence of the current should be calculated for each link separately and have derived a discrete analogue of Gauss' divergence theorem. We have also explained why the link current is more physically meaningful than the point current and, using the discrete divergence theorem, have shown that the difference arises in the discretization process itself. Hence we have demonstrated that discrete models, whether single-component (e.g. the finite-difference Schrödinger equation) or multi-component (e.g., multi-band tight-binding models), share common features: that currents are only defined along

links and that the link current is the physically relevant discrete current. Finally, using these results we have demonstrated the point form of probability conservation for a discrete model with a general, multi-component basis, deployed on an arbitrary mesh.

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