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Electronic states in continuous random networks: Rivier lines as half-integer magnetic flux lines

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We develop a simple effective-mass formalism for studying the effect of the Rivier lines (odd lines) on the electronic states in a tight-binding model defined for continuous random networks. Rivier lines act like infinitely thin fictitious solenoids carrying half-integer magnetic flux quanta for states close to the antibonding end of the band. The electron feels the effect of these flux lines through a "vector potential." Half-integer flux quanta of the flux lines ensure time-reversal invariance of the Hamiltonian. We briefly discuss some consequences of the peculiar properties of the Rivier lines and applications of our effective-mass formalism.

I. INTRODUCTION

In this paper we study some aspects of the electronic states in a tight-binding model defined on a continuous random network (CRN).[1] These types of networks have been studied in detail[2–5] to understand the electronic structures of amorphous materials such as *a*-Ge, *a*-Si, and glassy network materials. These studies have shown that topological disorder can sustain well-defined band gaps, sharp band edges, as well as bring in localized states.[2] The localization in these models is not merely due to simple potential fluctuation. It also arises due to interference from the Rivier lines,[6] which are the nontrivial topological content of a seemingly random network. It is known that the Rivier lines do not affect qualitatively one end of the band corresponding to the long-wavelength (bonding) electronic states. The other end of the band, which corresponds to the antibonding states, is severely affected and localized states are created. This has been demonstrated in detail in the recent works.[3–5] There is some experimental evidence for the presence of Rivier lines in amorphous materials.[7] How close the actual structures are to CRN is still under debate.[8]

Our aim in the present paper is to set up a simple formalism which can be used to study the effect of Rivier lines quantitatively, at least close to the band edges. To this end, we derive an-effective mass equation and show that the effect of the Rivier lines appear in a nontrivial way through some magnetic vector potential. This magnetic vector potential arises from the Rivier lines which behave like infinitely thin fictitious solenoids carrying half-integer magnetic flux quanta. The time-reversal invariance of the Hamiltonian is preserved because the flux lines carry half-integer flux quanta. We discuss at the end of the paper how our formalism paves the way for the study of the effects of Rivier lines on impurity states and exciton states in amorphous semiconductors. We also point out a possibility recently studied by the present author and Y. Fu,[9] namely, the topologically induced charges along the Rivier lines. There is some connection between our work and the earlier works of Gutzwiller and Wells, and Kawamura and co-workers[10–12] regarding the electronic states in the presence of dislocations in crystalline materials. However, there are important differences and new aspects which we discuss at the end. The connection of Rivier lines to Toulose lines[13] which appear in the short-range Ising spin-glasses is also discussed toward the end of this paper. The vector potential that appears in the present problem has a connection to the gauge fields introduced phenomenologically by Hertz[14] to take into account the effects of frustrations in a theory of spin-glass.

II. RIVIER LINES

Consider a continuous network. It has vertices (atoms) connected by bonds. A regular network like a cubic lattice or a diamond lattice contains elementary faces (or rings) formed out of an even number of atoms. When we consider a continuous random network (for example, every atom containing the same coordination number), there are in general odd numbered rings as well as even numbered rings. Rivier[6] showed that the odd numbered rings cannot occur in isolation, due to simple topological constraints. They occur in such a way that we can thread a continuous line through the odd rings without passing through any of the even rings. These lines should be closed or end at the surface of the network. These are called Rivier lines or odd lines.

The proof for the presence and the properties of Rivier lines is as follows. Consider an elementary volume in the network—called Euler cells. By definition, elementary volumes are made up of elementary faces and do not contain any atoms inside. If any faces of an elementary volume contain odd numbered rings, they have to occur in pairs. This follows from the fact that every edge of the cell is shared by two faces (rings). Thus, if a Rivier line enters an elementary volume it also has to leave it. In other words, Rivier lines cannot have ends. The above is analogous to a discrete version of Gauss's law.

A general continuous random network contains a finite density of Rivier lines of varying shapes and lengths randomly distributed in the network. If we consider a periodic network like an fcc lattice, we notice that it also

has Rivier lines. But these Rivier lines form a periodic network. The analogue of the Rivier line in two dimensions is the Rivier point. A simple example is a two-dimensional triangular lattice. Every elementary plaquette is a Rivier point: it is an odd ring with three atoms.

The presence of Rivier lines indicates the presence of "frustration" in the following sense.[3-5] Suppose we want to build antibonding eigenstates on one end of the band in a tight-binding model. This is possible in a bipartite lattice like a cubic or a bcc lattice (or a random network without any frustration). This is not possible in the presence of Rivier lines. The antibonding requirement cannot be satisfied along closed rings enclosing an odd number of Rivier lines. This means that along some surface bounded by the Rivier lines the eigenfunction will have bonding character. This is the origin of frustration in this context.

III. EFFECTIVE-MASS EQUATION

Consider a tight-binding model defined on a network. Every vertex in the network carries an orbital with zero energy. There is a hopping matrix element t_{ij} between any two vertices connected by a bond in the network. The Hamiltonian of the system is

$$H=\sum t_{ij}(\psi_i^\dagger\psi_j+\text{H.c.})\ , \tag{3.1}$$

where $t_{ii}=0$, $t_{ij}\geq 0$ and $(\psi_i^\dagger,\psi_i)$ are the creation and annihilation operators for electrons at the ith orbital. If the network is regular and unfrustrated, the density of states $\rho(\epsilon)$ of energy eigenvalue ϵ is symmetric:

$$\rho(\epsilon)=\rho(-\epsilon)\ .$$

This follows from that fact that any unfrustrated network can be separated into two sublattices A and B. The following transformation,

$$(\psi_i^\dagger,\psi_i)\rightarrow(-\psi_i^\dagger,-\psi_i)\ , \tag{3.2}$$

for all i belonging to one sublattice (say A), transforms the Hamiltonian $H\rightarrow -H$ and hence $\rho(\epsilon)=\rho(-\epsilon)$.

A network containing Rivier lines cannot be separated into two sublattices and hence the above transformation does not work. So

$$\rho(\epsilon)\neq\rho(-\epsilon)\ .$$

Physically it amounts to the fact that since on the antibonding side of the band the antibonding is not satisfied everywhere, there is a decrease in the energy of the eigenstates compared to the unfrustrated case. Antibonding requirements are satisfied in isolated regions free of Rivier lines, which gives rise to a Lifshitz tail of localized states.[3-5]

The effective-mass equation for the lower end of the spectrum has been discussed by Cohen.[5] The Rivier lines do not give rise to any qualitative change. The long-wavelength states are relatively unaffected. The effective-mass equation is the Schrödinger equation of a free particle. Now, we derive the effective-mass equation for the high-energy side of the band. This is not straightforward due to the presence of the Rivier lines.

The high-energy side of the spectrum of H is the same as the low-energy spectrum of $-H$. Hence, we define

$$H_R\equiv -H=-\sum\tilde{t}_{ij}(\psi_i^\dagger\psi_j+\text{H.c.})\ , \tag{3.3}$$

where $\tilde{t}_{ij}\equiv -t_{ij}$. We will study the low-energy side of the Hamiltonian H_R.

The Hamiltonian H_R has the following local symmetry: the transformations

$$(\psi_i,\psi_i^\dagger)\rightarrow(\psi_i e^{i\theta_i},\psi_i^\dagger e^{-i\theta_i}) \tag{3.4}$$

and

$$\tilde{t}_{ij}\rightarrow\tilde{t}_{ij}e^{i(\theta_i-\theta_j)} \tag{3.5}$$

leave the Hamiltonian invariant. Here, θ_i is an arbitrary function of the site i. This continuous symmetry of the Hamiltonian is analogous to the discrete symmetry of the Ising spin-glass Hamiltonian discussed by Toulose.[13] Let us formally rewrite the negative sign associated with every bond as

$$\tilde{t}_{ij}=t_{ij}\exp\left[i\int_i^j\mathbf{A}\cdot d\mathbf{l}\right]\ , \tag{3.6}$$

where the vector $\mathbf{A}(\mathbf{r})$ is a function of the spacial coordinate $\mathbf{r}$. Then the transformation of $\tilde{t}_{ij}$ [Eq. (3.5)] can be thought of as arising from the following transformation:

$$\mathbf{A}\rightarrow\mathbf{A}+\nabla\theta\ , \tag{3.7}$$

such that

$$\int_i^j\nabla\theta\cdot d\mathbf{l}=\theta_i-\theta_j\ . \tag{3.8}$$

Also the product of the sign of $\tilde{t}_{ij}$ along a closed loop C,

$$\prod_{ij\in C}\text{sgn}(\tilde{t}_{ij})=\exp\left[i\oint_C\mathbf{A}\cdot d\mathbf{l})\right)=\pm 1\ , \tag{3.9}$$

depending on whether C encloses an even number or odd number of Rivier lines. This follows that fact that, by definition, any closed ring that encloses an odd (even) number of Rivier lines contains an odd (even) number of bonds. The above product is also invariant under the local transformation defined in Eq. (3.7).

Because of the transformation property [Eq. (3.7)] and the invariance property of Eq. (3.9), the phase factor $\exp(i\int_i^j\mathbf{A}\cdot d\mathbf{l})$ attached to every bond behaves exactly like the effect of a vector potential on a charged particle in a tight-binding model.[15] A vector potential satisfying Eq. (3.10) is produced precisely by an infinitely thin solenoid carrying half-integer flux quanta and running along the Rivier lines. Once we realize the above, the continuum or the effective-mass approximation is straightforward.

First, we consider the case without the vector potential. We imagine $\psi(\mathbf{r})$ to be defined at every point. And $\psi_i\equiv\psi(\mathbf{R}_i)$. We can expand $\psi(\mathbf{R}_j)$ around $\mathbf{R}_i$ to get

$$\psi_j\approx\psi(\mathbf{R}_i)+(\mathbf{R}_j-\mathbf{R}_i)_\mu\partial_\mu\psi(\mathbf{R}_i)+\tfrac{1}{2}(\mathbf{R}_j-\mathbf{R}_i)_\mu(\mathbf{R}_j-\mathbf{R}_i)_\nu\partial_\mu\partial_\nu\psi(\mathbf{R}_i)+\cdots\ . \tag{3.10}$$

Substituting this in the Hamiltonian H_R we get

$$H_R \approx -\int d\mathbf{r}\frac{\hbar^2}{2m^*_{\mu\nu}(\mathbf{r})}\psi^\dagger(\mathbf{r})\partial_\mu\partial_\nu\psi(\mathbf{r})dr + \int d\mathbf{r}V(\mathbf{r})\psi^\dagger(\mathbf{r})\psi(\mathbf{r}) , \tag{3.11}$$

where

$$V(\mathbf{r})=\sum_j t_{ij}\delta(\mathbf{r}-\mathbf{R}_i) \tag{3.12}$$

and

$$\frac{\hbar^2}{2m^*_{\mu\nu}(\mathbf{r})}=\sum_j t_{ij}(\mathbf{R}_i-\mathbf{R}_j)_\mu(\mathbf{R}_i-\mathbf{R}_j)_\nu\delta(\mathbf{r}-\mathbf{R}_i) . \tag{3.13}$$

In the effective-mass approximation for the random system we expand the potential [Eq. (3.12)] and the effective mass [Eq. (3.13)] in a Fourier series and keep essentially the small momentum components below a momentum cutoff Λ as follows:

$$\tilde{V}(\mathbf{r})=\sum_{\mathbf{q}}\exp(-q/\Lambda)V(\mathbf{q}) , \tag{3.14}$$

$$\tilde{m}^*(\mathbf{r})=\sum_{\mathbf{q}}\exp(-q/\Lambda)m^*(\mathbf{q}) , \tag{3.15}$$

where $m^*(\mathbf{q})$ and $V(\mathbf{q})$ are the Fourier coefficients of the effective mass and the potential. Thus, the single-particle effective-mass Hamiltonian is

$$H_{\text{eff}}=-\frac{\hbar^2}{2\tilde{m}^*_{\mu\nu}(\mathbf{r})}\partial_\mu\partial_\nu+V(\mathbf{r}) . \tag{3.16}$$

The eigenfunctions of the above effective-mass Hamiltonian are a good approximation to the actual eigenfunctions, as long as the spatial variation of the solution is at a length scale which is large compared to Λ^{-1}.

We see from Eqs. (3.12) and (3.13) that the spatial variation and the anisotropy arise from the fluctuation in the matrix elements, as well as from the fluctuation in the coordination numbers. When we want to consider the effects arising from bond-angle, bond-length, and dihedral-angle fluctuations, we have to keep the spatial dependence. When there is no localization caused by these fluctuations, the anisotropy and spatial dependence of the effective mass are not very important.

The effect of the vector potential is easily included. Now, we expand $\psi_j\exp(i\int_i^j \mathbf{A}\cdot d\mathbf{l})$ about $\mathbf{R}_i$ and keep terms only up to the second derivative in ψ's and the first derivative in $\mathbf{A}$. When we neglect the anisotropy and spatial dependence of the effective mass, the path-dependent phase factor just adds the vector potential to the momentum in the usual fashion. Thus, the single-particle effective-mass Hamiltonian for the antibonding side of the band is

$$H_{\text{eff}}=\frac{-\hbar^2}{2\tilde{m}^*}[\nabla+i\mathbf{A}(\mathbf{r})]^2+\tilde{V}(\mathbf{r}) , \tag{3.17}$$

where $\mathbf{A}(\mathbf{r})$ satisfies Eq. (3.10). Alternatively, $\mathbf{A}$ also satisfies the differential equation

$$\nabla\times\mathbf{A}=\mathbf{h} , \tag{3.18}$$

where $\mathbf{h}(\mathbf{r})$ is the "magnetic field" which is nonzero only along the solenoid. Notice that since there is no physical magnetic field in the problem the electronic charge and velocity of light do not appear along with the vector potential. The eigenfunctions of the effective-mass equation (3.17) are the envelope functions of the antibonding wave function in our tight-binding model.

We can use the similarity of Eq. (3.18) to a Maxwell equation that relates magnetic field and current (Biot Savart law) to write the solution

$$\mathbf{A}(\mathbf{r})=-\frac{1}{8\pi}\int_\Omega\frac{\mathbf{R}\times d\mathbf{S}}{R^3} , \tag{3.19}$$

where $d\mathbf{S}$ is the differential element of the Rivier lines Ω and $\mathbf{R}$ is the distance of the point $\mathbf{r}$ to the differential element.

The Hamiltonian is time-reversal invariant. Under the time-reversal transformation, ∇ changes sign. The vector potential remains unchanged in this transformation. The change in sign of ∇ can be compensated for by adding a term $2i\mathbf{A}(\mathbf{r})$ to the vector potential. This amounts to adding a unit flux quantum to every flux line. According to the Aharanov Bohm effect, this does not change the physics of the problem,[16] and hence the time-reversal invariance.

Since the vector potential due to the Rivier lines is curl free everywhere except on the Rivier lines, we can even eliminate the vector potential from the Schrödinger equation by a singular gauge transformation and include its effect through the boundary condition on the wave function. That is, after the elimination, the Schrödinger equation is

$$-\frac{\hbar^2}{2\tilde{m}^*}\nabla^2\psi+\tilde{V}(\mathbf{r})=E\psi , \tag{3.20}$$

with the boundary condition that the solution should change sign if we take the coordinate around any closed path which encloses an odd number of Rivier lines.

Now, we can make several comments about the effect of Rivier lines. Firstly, Rivier lines produce nontrivial momentum-dependent potentials through the vector potential. The effect of the vector potential cannot be treated by simple perturbation theory. As an example we give the effect of a simple Rivier line on the electronic states.

Assume that we have only one Rivier line running along the z axis. Its vector potential has a simple form

$$\mathbf{A}(\rho)=\frac{\hat{\theta}}{2\rho} \tag{3.21}$$

in cylindrical polar coordinates. The effective-mass equation has the form

$$-\frac{\hbar^2}{2m^*}\left[\frac{\partial^2\psi}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial\psi}{\partial\rho}+\frac{\partial^2\psi}{\partial z^2}+\frac{1}{\rho^2}\left[i\frac{\partial}{\partial\theta}+\frac{1}{2}\right]^2\psi\right]=E\psi . \tag{3.22}$$

Consider the scattering of a plane wave with momentum along the positive x axis. The analysis is straightforward and we can use the known results from the scattering of electrons by thin flux lines.[16] The waves scattered by the flux lines interfere strongly, which results in the vanishing

of the wave function in the complete z-x plane to the right of the z axis. This vanishing happens precisely when the flux is half the flux quanta. This has an interesting consequence for our problem. If we have a large Rivier line forming a closed loop, the eigenfunctions have to vanish along a surface bounded by the loop. In our tight-binding model this means that the eigenfunction will have bonding character along a plane of atoms bounded by the Rivier line.

The scattering of electrons by the above Rivier line can also be easily calculated to get the expression for the scattering matrix,

$$t(\mathbf{k},\mathbf{k}')=-i\frac{\hbar^2}{\tilde{m}^*}\frac{e^{\pm i\theta_{kk'}}}{\sin(\theta_{kk'}/2)}\ , \tag{3.23}$$

where $\mathbf{k}$ and $\mathbf{k}'$ are the incident and scattered wave vectors and $\theta_{kk'}$ is the angle between them. Similar examples can be obtained for scattering from a circular Rivier line as well as some more complicated geometries using known results of scattering electrons by magnetic flux lines.[17] These scattering matrix elements will be useful for calculating the relaxation time of carriers, as well as for developing a scaling theory of localization on the antibonding end of the band.

IV. RIVIER LINES IN REGULAR LATTICES

Tight-binding models with random transfer integrals have been studied by some authors.[18] We show that these models have the same physics as the tight-binding model in a CRN but with no randomness in the sign of the transfer integrals. We show that a nontrivial content of both are Rivier lines. However, there is one important difference in this case, namely, both ends of the bands are affected by the Rivier lines. This discussion also brings in the close connection between the Rivier lines and Toulose lines.[13]

Consider a simple-cubic lattice with nearest-neighbor hopping t_{ij}, which can take two values ± 1 with some probability. When we consider a particular configuration of hopping matrix elements, we can define the so-called frustration function as the product of the sign of the t_{ij} around every elementary plaquette p:

$$\Phi_p=\prod_p \mathrm{sgn}(t_{ij})\ . \tag{4.1}$$

The plaquette is frustrated if Φ_p is negative and not frustrated if it is positive. It has been shown by Toulose that the frustrated plaquettes cannot occur in isolation.[13] A continuous line can be thread through them without crossing unfrustrated plaquettes. These are essentially the Rivier lines of this topologically regular network. Even though from the geometry we can form a perfect bonding and antibonding state in this lattice, they are not eigenstates of the Hamiltonian in general, due to the random sign of t_{ij}. Frustration arises when we try to build an eigenstate, taking care of the sign of t_{ij} as well. In this case it is easily seen that both sides of the bands are affected by the Rivier lines. In fact, the effective-mass equation contains the same vector potential due to the Rivier lines on both sides of the band.

V. APPLICATIONS

A. Real systems

In this section we briefly discuss various possible applications of the effective-mass theory. Firstly, how relevant is the above discussion for real systems such as a-Ge and a-Si? The electronic structure of a-Ge and a-Si in a CRN model has been studied by several authors. Recently, Singh[3] carried out this investigation in great detail, both analytically and numerically. The basis of this model is that each site carries four optimally localized orbitals. One of them is an s orbital and the others are the p orbitals. There are several hopping matrix elements: on-site hopping between different orbitals and nearest-neighbor hopping. The bond-length, bond-angle, and dihedral-angle fluctuations add randomness to the transfer integrals. It has been argued that the Rivier lines have an important effect on some region in the band.[5] As has been discussed by Cohen and co-workers, the basic effect of odd rings is similar to the one-orbital model that we have discussed so far. The details differ because of the presence of the many orbitals. However, when one considers states close to the top of the valence band or bottom of the conduction band, states are predominantly formed by simple hybridized orbitals from neighboring sites. In the case of Si the bottom of the conduction band corresponds to antibonding states formed by hybridized $SP\delta$ orbitals. In these cases the effective-mass equation contains the vector potential. The multivalley nature of the bands can also be taken care of in principle through the modification of the effective-mass equation, as in the crystalline semiconductors.

B. Impurity states in semiconductors

In a semiconductor, shallow donor or acceptor impurity states are formed predominantly using states close to the bottom of the conduction band or the top of the valence band. Thus, effective-mass approximation is very useful for understanding the properties of the impurity states. As discussed above, the effect of Rivier lines appears through a vector potential, depending on whether the corresponding band edge is of the antibonding type or not. Neglecting the local potential fluctuations and the mass anisotropy, the effective-mass equation has the following form:

$$-\frac{\hbar^2}{2\tilde{m}^*}(\nabla-i\mathbf{A})^2\psi+V_I(\mathbf{r})\psi=E\psi\ , \tag{5.1}$$

where $V_I(\mathbf{r})$ is the screened impurity potential. If the Rivier line passes in the vicinity of the impurity (within the effective Bohr radius), it has a strong influence on the impurity eigenstates. As we saw earlier, the wave function becomes zero along a plane emanating from the Rivier line. Simple estimates[19] show that this changes the energy levels appreciably. In a real semiconductor, since impurities are distributed randomly, what one observes experimentally will be an averaged effect.

C. Excitons

The effect on Wannier excitons is very similar to the effect on impurity states. In general, the hole states and electron states are not affected by the Rivier lines in the same way. As we mentioned earlier, in Si the electron states near the bottom of the conduction band are affected by the Rivier lines more than the hole states at the top of the valence band. Thus, in the effective-mass equation, the electron is affected by a vector potential, whereas the hole is not affected by any vector potential. This makes the study of excitons in the presence of Rivier lines interesting and rich.

D. Induced charge along the Rivier lines

Recently, the present author and Y. Fu[9] have shown that under some conditions fractional charges can be induced along the Rivier lines. This arises because the Rivier lines are topologically nontrivial objects. Thus, if we compare the Fermi sea of electrons with the Fermi level lying in a band gap or mobility gap in some specific tight-binding models, the eigenstates are affected in an essential way before and after the introduction of the Rivier lines into the system. By the same physics that produces charge depletion or excess charge in a domain wall in polyacetylene,[20] we also get excess charge distributed along the Rivier lines under some conditions. This could be one of the origins[9] of the strong internal electric fields observed experimentally in glassy materials.

VI. DISCUSSION

In this paper we discussed how Rivier lines affect the electronic states of simple tight-binding models in CRN. We showed that a Rivier line plays the role of an infinitely thin solenoid carrying a half magnetic flux quantum. We argued that the resulting effective-mass equation will be useful in discussing some important questions in amorphous semiconductors like the impurity states, exciton states, etc. Since Rivier lines are of topological origin, electron-phonon, as well as electron-electron interaction, cannot qualitatively change its effect.

Topologically nontrivial defects like screw dislocations in crystalline materials have been shown by some authors[10–12] to affect the electronic states in a nontrivial way. For example, it was shown that if one considers a screw dislocation in a simple-cubic lattice along the z axis, it acts like a magnetic flux line. But the magnitude of the flux line is not a constant. It depends on the z-component momentum of the electron. In this sense these fluxes are more complicated than the flux lines discussed by us. This is consistent with an important point raised by Rivier that dislocations are fundamentally differential from the dislocations in crystals. Moreover, the present author has shown that if one considers the electronic states on the high-energy end of the band for a dislocated crystalline lattice the dislocation line also acts like an odd line.[19] It contributes a half flux quantum in addition to the usual flux discussed by the above authors.

Tight-binding networks in the presence of magnetic fields have been studied recently in the context of granular superconductors, Josephson-junction networks, and localization problems in strong magnetic fields. We have shown in the present paper that frustration can provide a restricted class of desired magnetic fields. To give an example, recently Fisher and Fradkin[21] studied the localization problem in a square lattice in the presence of a strong magnetic field, such that each plaquette encloses half a flux quantum. As mentioned by these authors, this requires astronomically large fields. A study of our paper reveals that this situation can be studied without any external field by a proper choice of layered compound in two dimensions. Frustration provides us the required half flux quanta. It is easily seen that the effect of the half flux quanta of Fisher and Fradkin can be simulated by changing the sign of every other hopping integral in the y direction. Of course, such a system may be very difficult to synthesize. However, the same physics can be studied by considering a tight-binding system in a triangular lattice in two dimensions and by studying the appropriate end of the band.

Hertz[14] introduced gauge fields to take into account the effect of the frustrations in spin-glasses in a Landau free energy in a phenomenological way. Our work provides the explicit form of the gauge field. This is because the matrix of the exchange interaction between the spins is analogous to the tight-binding matrix, and the gradient term appearing in the Landau free-energy function is analogous to the kinetic energy term appearing in the effective-mass equation.

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