QUANTUM TRANSPORT AND COHERENCE IN BOUNDARY LIMITED ELECTRONIC DEVICES: RECURSIVE DYSON HAMILTONIAN GREEN'S FUNCTION AND FINITE ELEMENT TECHNIQUES IN HETEROSTRUCTURES

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Abstract

With the decreasing scale of electronic devices, increasing attention is being paid to the finite sized nature of the resulting structures. This necessitates particular efforts to take into account the constraining as well as limiting behavior of the device boundaries. Methods to efficiently formulate theoretically these effects, and then to construct user friendly, flexible, time efficient computer codes are becoming very important. Such issues will be addressed here as we discuss ballistic transport in 1D Aharonov - Bohm rings using a discrete tight - binding Hamiltonian, the 3D quantum transmission into and out of a multiport cavity in the linear single - particle weak - like variational formulation, and the nature of the above techniques in view of general variational and weighted residual techniques possible for extremely general media found in microwave and electromagnetic problems .

I. TRANSPORT IN 1D AHARONOV-BOHM HETEROSTRUCTURE RINGS

Electron transport through quantum interference device-like structures is of interest where microstructure fabrication allows multiple channels of quantum wave flow to occur. This is possible to achieve in finite width heterostructure waveguides. For narrow width channels, the channels may be considered 1D chains and analyzed in discretized form using tight-binding functions [1]. Non-local vector potential effects will alter relative phase information in the electron wave functions and cause varying interference behavior at channel intersections. For wide channels this tight-binding Hamiltonian technique, which yields recursive Green's functions, may not be the best way to approach the 2D nature of the problem. Finite element techniques which can easily allow for finite wall locations and arbitrary geometries may be a much more general method based upon solving the suite of physical field and transport governing equations. Section II discusses that method appropriate for 3D problems.

An infinite chain is intercepted at sites 0 and (N + 1) by a finite loop, with N' sites. By choosing a symmetric gauge, the vector potential, $\mathbf{A}(\mathbf{r})$ is given by:

$$\mathbf{A}(\mathbf{r}) = \frac{1}{2}\mathbf{H}\times\mathbf{r} \tag{1}$$

By the use of Peierl's substitution [2], the hopping potential which appears in the tight-binding Hamiltonian, becomes (h is Planck's costant divided by 2π):

$$\hat{V}_{ij} \rightarrow V\exp\left(\frac{ie}{hc}\mathbf{A}(\mathbf{r}_i)\cdot\mathbf{r}_j\right) \tag{2a}$$

Upon substitution of (1) and (2), and using well known vector identies, we find:

$$\hat{V}_{ij} = V\exp\left(\frac{ie}{hc}\frac{1}{2}\mathbf{H}\times\mathbf{r}_i\cdot\mathbf{r}_j\right) = V\exp\left(\frac{ie}{2hc}\mathbf{H}\cdot\mathbf{r}_i\times\mathbf{r}_j\right) \tag{2b}$$

Here, V_{ij} represents the hopping matrix element in a nearest-neighbor tight-binding formulation, so that $V_{ij} \neq 0$ for $i = j \pm 1$, and $= 0$ otherwise. To compute the effect of the loop induced scattering on the transmission amplitude, we use Dyson's equation [3]. $G_0(n, m)$ represents the

$$G(\alpha, \beta) = G_0(\alpha, \beta) + G_0(\alpha, 0)\hat{V}(0, 1')G(1', \beta) + G_0(\alpha, N+1)\hat{V}(N+1, N')G(N', \beta) \quad (3)$$

α an β indicate respectively the extreme left and right of the infinite chain, primes denote the loop locations, and 0 and $N + 1$ indicate respectively the intersections of the infinite chain and loop at the left and right. Unlike the field-free case [3],

$$\hat{V}(i, j) = \left[\hat{V}(j, i)\right]^* \quad (4)$$

We start the derivation with the propagator for an infinite one-dimensional tight-binding chain [4]:

$$G(1, m; z = E) = \left[2V\sqrt{1 - \left(\frac{E}{2V}\right)^2}\right]^{-1}\left[\frac{E}{2V} + i\sqrt{1 - \left(\frac{E}{2V}\right)^2}\right]^{|1-m|} \quad (5)$$

where we have used $E = 2V\cos ka$ for a tight-binding band, the site energy E_0 being set arbitrarily to zero. Setting $ka = \theta$, we find $E/2V = \cos\theta$, which yields:

$$G_0(1, m; E) = \frac{i}{2V\sin\theta}(\cos\theta + i\sin\theta)^{|1-m|} = \frac{ie^{i|1-m|\theta}}{2V\sin\theta} = G(0, 0; E)e^{i|1-m|\theta} \quad (6)$$

For a tight-binding chain of atoms, we start with a single site and add sites iteratively through the Dyson equation. For a single site [4],

$$G_0(1, 1; E) = \frac{1}{E} = \frac{1}{2V\cos\theta} \quad (7)$$

For two sites, we write the basic Dyson equation (previously used to generate equation (3)), where G_0 = Green function for the single site, and G = Green function for the two sites, and $\hat{V}$ = the hopping matrix element between the two sites:

$$G = G_0 + G_0\hat{V}G \quad (8)$$

Then applying (8) to both the diagonal and off-diagonal matrix element:

$$G(1, 1) = G_0(1, 1) + G_0(1, 1)\hat{V}_{12}G(2, 1) \quad (9a)$$

$$G(2, 1) = 0 + G_0(2, 2)\hat{V}_{21}G(1, 1) \quad (9b)$$

Substituting (9b) into (9a), we obtain:

$$G(1, 1)\left[1 - G_0(1, 1)\hat{V}_{12}G_0(2, 2)\hat{V}_{21}\right] = G_0(1, 1)$$

$$G(1, 1) = \frac{G_0(1, 1)}{1 - V^2G_0(1, 1)G_0(2, 2)} = \frac{1}{2V\cos\theta}\frac{4\cos^4\theta}{4\cos^2\theta - 1} = \frac{\sin 2\theta}{V\sin 3\theta} \quad (10)$$

Notice that the phase factors found in the hopping matrix elements in (2) cancel out in the (10) expression. To find the off-diagonal matrix element G(1, 2) we again write:

$$G(1, 2) = G_0(1, 1)\hat{V}_{12}G(2, 2) \quad (11a)$$

$$G(2, 2) = G_0(2, 2) + G_0(2, 2)\hat{V}_{21}G(1, 2) \quad (11b)$$

Substituting (11b) into (11a),

$$G(1, 2) = \frac{G_0(1, 1)\hat{V}_{12}G_0(2, 2)}{1 - V^2G_0(1, 1)G_0(2, 2)} = \frac{V\exp\left(\frac{ie}{2hc}\mathbf{H}\cdot\mathbf{r}_1\times\mathbf{r}_2\right)\frac{1}{4V^2\cos^2\theta}4\cos^2\theta}{4\cos^2\theta - 1} = e^{i\gamma(1, 2)}\frac{\sin\theta}{\sin 3\theta} \quad (12)$$

where the argument of the phase factor has been replaced by $\gamma(1, 2)$.

For finite chains of arbitrary length N, we use the results for one and two sites and apply a recursive Green's function technique [5] to generate further sites. Continuation of this process leads to finding the transmission amplitude.

The transmission amplitude, t, is defined by:

The transmission amplitude, t, is defined by:

$$t = \frac{G(\alpha, \beta)}{G_0(\alpha, \beta)} = \frac{\text{amplitude for propagation through whole structure}}{\text{amplitude without upper loop}} \tag{13}$$

while the transmission coefficient is,

$$T_{NN'}(E, \phi) = t \cdot t^* \tag{14}$$

where E is the energy of the incident electron and ϕ is the ratio of the flux enclosed by the loop to the flux quantum $\phi_0 = hc/e$. The final result for $T_{NN'}(E, \phi)$ is:

$$T_{NN'}(E, \phi) = 4\left[\cos^2\frac{\phi}{2}\sin^2\alpha\cos^2\beta + \sin^2\frac{\phi}{2}\sin^2\beta\cos^2\alpha\right]\times$$
$$\left\{\left[\sin(2\alpha) + \cot\theta(\cos^2\alpha - \cos^2\beta)\right]^2 + \left[\cos\phi + 1 + \cot\theta\sin(2\alpha) - \left(3 - \frac{1}{2\sin^2\theta}\right)\cos^2\alpha - \left(\frac{1}{2\sin^2\theta} - 1\right)\cos^2\beta\right]\right\}^{-1} \tag{15}$$

where

$$\alpha = \frac{N + N' + 2}{2}\theta \tag{16a}$$

$$\beta = \frac{N' - N}{2}\theta \tag{16b}$$

and where θ is related to the energy in a single tight-binding band:

$$E = 2V\cos\theta \tag{17}$$

It can be verified easily that (15) reproduces the result for the field-free case derived by Ginuea and Verges [3] when $\phi = 0$.

II. 2D AND 3D MODELLING OF ELECTRON WAVE PROPAGATION IN HETEROSTRUCTURE DEVICES USING FINITE ELEMENTS

The description starts with the Schrodinger equation in 3D

$$-\frac{h^2}{2m}\left(\hat{\mathbf{P}} - \frac{e}{c}\mathbf{A}\right)^2\Psi(x, y, z) + V(x, y, z)\Psi(x, y, z) = E\Psi(x, y, z) \tag{18}$$

where h is Planck's constant divided by 2π. For a uniform magnetic field, the gauge is nonunique which leads to a A choice. Following Wang et. al. [6], $\mathbf{A} = (-By/2, Bx/2)$ and

$$-\frac{h^2}{2m}\nabla^2\Psi(x, y, z) + \hat{V}(x, y, z)\Psi(x, y, z) = E\Psi(x, y, z)$$
$$\hat{V}(x, y, z) = V(x, y, z) - \frac{iehB}{2mc}\left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right) + \frac{e^2B^2}{8mc^2}(x^2 + y^2) \tag{19}$$

Performing the 3D integral over the device volume, with an input port on the left at $x = x_1$ and an output port at the bottom at $y = y_2$, and using Green's theorem,

$$\frac{h^2}{2m}\iiint_{\Omega_0}\nabla\tilde{\Psi}\cdot\nabla\Psi d\Omega + \iiint_{\Omega_0}\tilde{\Psi}(\hat{V} - E)\Psi d\Omega = \frac{h^2}{2m}\sum_{i=1}^{2}\oiint_{\Gamma_i}\tilde{\Psi}\nabla\Psi\cdot\hat{n}d\Gamma \tag{20}$$

Apply a finite element discretization in the cavity region.

$$\Psi(x, y, z) = N(x, y, z)U \quad ; \quad \tilde{\Psi}(x, y, z) = N(x, y, z)\tilde{U} \tag{21}$$

Here N(x, y, z) is the global shape function, U is a vector of all the unknown wave function Ψ values on the nodes, and U tilde the trial U. Then (20) becomes

$$\tilde{U}(T + V)U = \frac{h^2}{2m}\sum_{i=1}^{2}\oiint_{\Gamma_i}\tilde{\Psi}\nabla\Psi\cdot\hat{n}d\Gamma \tag{22}$$

The surface integral in (22) which includes a depth d in the z-direction, requires a minor modification to convert from a line to a surface integral. The result is

$$\tilde{U}(T + V)U = \tilde{U}_1P - \tilde{U}_1C^1U_1 - \tilde{U}_2C^2U_2 \tag{23}$$

where

$$P_i = -\frac{h^2}{2m}\oiint_{\Gamma_1}\phi_i^1(x, y, z)\left[\mathbf{h}^1(y, z) - \mathbf{h}^2(y, z)S^{-1}\tilde{S}\right]ad\Gamma \tag{24}$$

$$C_{ij}^1 = \frac{h^2}{2m}\oiint_{\Gamma_1}\phi_i^1(x, y, z)\sum_{m, n}h_m^2(y, z)S_{mn}^{-1}T_{nj}^1d\Gamma \tag{25}$$

$$C_{ij}^2 = \frac{h^2}{2m}\oiint_{\Gamma_2}\phi_i^2(x, y, z)\sum_{m, n}g_m(x, z)R_{mn}^{-1}T_{nj}^1d\Gamma \tag{26}$$

In (23), U_1 and U_2 only correspond respectively to the subset of nodes on port surfaces 1 and 2. Since P_i is known due to the specified incident wave amplitude vector **a**, we know that the partial global vectors U_1 and U_2 can be moved to the left hand side of (23) after proper assembly procedure [7] and [8]

$$\tilde{U}_1^TP = \tilde{U}^T\tilde{P} \quad ; \quad \tilde{U}_1^TC^1U_1 = \tilde{U}^T\tilde{C}^1U \quad ; \quad \tilde{U}_2^TC^2U_2 = \tilde{U}^T\tilde{C}^2U \tag{27}$$

as done in [9] and [10]. The solution follows immediately.

$$(T + V + \tilde{C}^1 + \tilde{C}^2)U = P \tag{28}$$

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