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Microelectronics Journal 36 (2005) 876–881

Microelectronics
Journal

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Why green functions for matching?

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Available online 1 July 2005

Abstract

Work on Surface Green Function Matching (SGFM) has been the subject of extensive collaborations with members of the Iberoamerican community of solid state physicists. The conceptual frame, the basic general results and their meaning, form and generality of scope are discussed. The practical aspects of SGFM calculations are discussed, with attention to formal arguments which prove useful in practice and to computational transfer matrix techniques. A wide range of selected applications are presented. The approach taken is a historical—not strictly chronological—perspective with emphasis on the significance of the results in their own time, as well as a reflection of the collaborations with many members of this community.

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1. Preliminary note

In the realm of linear differential equations a Green function is the *resolvent* of a differential system with given boundary conditions and this makes it a very useful object in physics. The Green function (GF) contains all the physical information on the system. It is also an object which admits appealing intuitive interpretations as a propagator or an input–output response function and it is neither more nor less difficult to calculate with GFs than with wavefunctions—or similar amplitudes. Moreover, GF techniques can be equally set up to study systems of finite difference equations which describe another class of physical models. GFs are, therefore, very useful objects in physics. We shall discuss here their role in matching problems—surfaces and/or interfaces.

GFs can be used, obviously, in different ways to solve matching problems. Two of them, in particular [1,2], have interesting immediate connections with the approach presently described. In this talk we shall discuss the basic ideas and main developments of an approach, the Surface Green Function Matching (SGFM) method, which has very largely taken place within the community represented in this symposium.

All technical details and formal arguments up to 1991 can be found in a book [3] and all developments up to 1993 are reviewed in Ref. [4]. Except for some later developments, all appropriate references are given in these two publications and need not be repeated here.

2. SGFM

Standard scattering theory, when cast in GF language, rests on Dyson's integral equation

$$G(\boldsymbol{r},r') = G_0(\boldsymbol{r},r') + \int d^3G(\boldsymbol{r},r'')V(r'')G_0(r'',r') \tag{1}$$

for the perturbed propagator G. If the scattering potential V is replaced by the (total scattering) 't matrix', then (1) can be cast, alternative and in compact notation, as

$$G = G_0 + G_0tG_0, \tag{2}$$

which is not yet a formula for G, as this depends on finding t, which is equivalent to solving the same integral equation.

Now consider two media, 1 and 2, described by corresponding GFs, G_1 and G_2, meeting at an interface which for the time being we shall assume to be a plane. The problem is to find G_S, the GF of the matched system 1/2 in terms of G_1 and G_2. After Fourier transform in the 2D surface plane, every G is a function $G(\kappa,\ \Omega;\ z,\ z')$ of the spatial coordinates z, z' normal to the surface, for given 2D wavevector κ and eigenvalue Ω which could be, for instance, the energy E for electronic states or ω^2 for elastic or electromagnetic waves.

We can look at the problem from a scattering theoretic viewpoint. Some elementary excitation which starts propagating from, say, r'_1 with unperturbed propagator G_1

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doi:10.1016/j.mejo.2005.05.005

will be perturbed—scattered—by the interface. Obviously we now have two classes of scattering events, namely, reflection and transmission. It is proved that the general form of the two basic matrix elements is

$$\langle 2|G_S|1'\rangle = \langle 2|G_1|1'\rangle + \langle 2|G_2|0\rangle\cdot\mathscr{R}\cdot\langle 0|G_1|1'\rangle \tag{3}$$

for reflection and

$$\langle 1|G_S|1'\rangle = \langle 1|G_1|0\rangle\cdot\mathscr{T}\cdot\langle 0|G_1|1'\rangle \tag{4}$$

for transmission. The alternative notation, e.g. $\langle 2|G|1'\rangle$ for $\langle z|G|z'\rangle$ when $z \subset 2$ and $z' \subset 1$ is selfexplanatory, $z=0$ or $z'=0$ denotes the position of the surface and we have introduced 2D *surface objects* like $\mathscr{R}$ and $\mathscr{T}$, defined to exists and have an inverse only in the surface plane. It is furthermore seen that

$$\mathscr{R} = \mathcal{G}^{-1}\cdot(\mathcal{G}_S - \mathcal{G}_1)\bullet\mathcal{G}^{-1}; \quad \mathscr{T} = \mathcal{G}_2^{-1}\cdot\mathcal{G}_S\cdot\mathcal{G}_1^{-1}. \tag{5}$$

The position is as with (2), only that now we have two '*t*-matrices', one for reflection and one for transmission. Note that the only unknown in (3) to (5) is $\mathcal{G}_S$. The central idea of SGFM is that all the physical information on the matched system is contained in $\mathcal{G}_S$, and this can be obtained in a formally exact manner from the matching conditions. The full $\mathcal{G}_S$ is then known and the scattering problem is turned into a matching problem, as the two '*t*-matrices', $\mathscr{R}$ and $\mathscr{T}$ are obtained from $\mathcal{G}_S$. All one has to do is to express appropriately the matching conditions.

In an elementary wavefunction analysis with a simple one band effective mass model, one matches the normal derivative—or logarithmic derivative—weighted with the inverse effective mass. The SGFM formulation requires attention to a technical detail. For a given medium ($j=1$, 2) we define the two—different—normal derivatives

$${}'\mathcal{G}^{j}_{\pm} = \lim_{z'\to\pm 0}\left[\frac{\partial G(z,z')}{\partial z}\right]_{z=0} \tag{6}$$

and then the weighted logarithmic derivatives

$$\mathcal{L}_j^{\pm} = \frac{1}{m_j}\,{}'\mathcal{G}^{j}_{\pm}\cdot\mathcal{G}_j^{-1}. \tag{7}$$

In the wavefunction analysis, on expressing the matching conditions one obtains a matching secular equation yielding the eigenvalues and corresponding eigenstates. In SGFM one obtains a formula—the matching formula—for $\mathcal{G}_S(\boldsymbol{\kappa}, E)$, namely

$$\mathcal{G}_S^{-1} = \frac{\hbar^2}{2}(\mathcal{L}_1^{+} - \mathcal{L}_2^{-}). \tag{8}$$

From this, one can obtain the matching secular equation as well as any other desired item of physical information, in particular, any spectral function of interest, and transmission and reflection amplitudes from (3) to (5).

SGFM first appeared in 1969, when surface states were being investigated in terms of simple models and it soon proved a useful tool for the exploration of some basic issues on which attention was at the time focused. Some emergent ideas turned out to be rather fruitful. It was soon realised that the Green function contains all the relevant physical information on the system, including that contained in the analytical continuation of the real energy band structure to complex k vectors. It was also seen that some key issues depend essentially on basic analytical properties of G_S as a function of the energy E, whether allowed or forbidden, and are therefore to some extend independent of details of the band structure. This allowed some of these basic issues to be clarified and significant progress to be made in terms of simple models, which was quite timely considering the rather modest computational facilities then available in most of our institutions.

We should consider the situation in those years. The idea of surface states was still somewhat vague. There was not even unanimous agreement about their actual existence, when some optical absorption experiments appeared as the first experimental evidence. A technical theoretical explanation was very timely to clinch the argument. We noted above that from $\mathcal{G}_S$ one can obtain the spectral functions of interest. An SGFM analysis with a very simple model of electronic structure established beyond doubt that the type of *van Hove* singularity which is unambiguously characteristic of a spectrum with a 2D quantum number checked with experimental evidence. The details of the optical absorption data might require a more elaborate model for a quantitative fit, but the topological argument is irrefutable. The observed absorption was due to transitions from occupied to unoccupied bands of surface states, both inside the optical gap of the 3D bulk band structure and both being bands of the form $E(\kappa)$ with κ 2D. The experiments in question could be said to have historical rank in the physics of surface states and, indeed, to constitute the first unmistakable evidence of their existence. In similar ways it was possible, for instance, to understand in simple terms the disappearance of surface states in *Si* as oxidation of the surface proceeds, to assess—and establish the limitations of—abrupt barrier models of the surface potential and to formulate the meaning and relevance of the concept of 'dangling bonds' in the frame of a theory of surface states.

Some basic aspects of the manybody interactions in the electron gas in the surface region were clarified, in particular the important role played by the concept of charge neutrality in the study of surfaces and interfaces. It was also possible to formulate a theory of tunnelling with no resort to a phenomenological tunnelling Hamiltonian, something allowed by the analytical properties of the Green function, i.e. the propagator. The relationship between $\mathcal{G}_S$ and $\mathscr{R}$ also allowed for a clarification of some basic aspects of LEED which depend on basic analytical aspects of $\mathcal{G}_S$ and not on details of the crystalline potential.

As time went on the use of more elaborate models of band structure became more generally accessible and further problems were successfully treated with SGFM, like some related to image states at metal surfaces, as well as the relevance for directional photoemission and others. But at this stage it is time to consider other aspects of SGFM.

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