# Comment on a recent theory of tunneling without the transfer-Hamiltonian formalism

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A comment is made about a recent paper by Feuchtwang. In particular, it is argued that the treatment of tunneling of Caroli *et al.*, as extended to the continuous limit, is exact, and that Feuchtwang's article, which leads to completely equivalent results, does actually confirm this statement.

In a recent paper,[1] Feuchtwang has proposed a new approach to the problem of tunneling in the independent-electron approximation. This treatment is, for such noninteracting systems, exact and free from the assumptions implied by the Bardeen transfer-Hamiltonian approach.

A similar formalism was constructed by our group some years ago,[2,3] and it was subsequently applied to various physical situations.[4] Feuchtwang makes a number of erroneous and highly misleading statements about our formulation in his paper, which in our opinion must be corrected.

Previous theories of tunneling were faced with two major difficulties: (i) how to construct a perturbation expression valid under nonequilibrium (albeit steady) conditions, as met when a finite bias is applied to a metal-insulator-metal junction; (ii) how to construct two complete sets of states separately for the left and right electrodes which, when taken together, (a) provide a complete set for the full system and (b) maintain a coupling between the electrodes.

The problem of completeness was raised long ago by Prange.[5] The situation with respect to problem (b) is obvious if one enforces the condition $\Psi = 0$ at the boundary between two *uncoupled* electrodes; with such wavefunctions, no current will ever flow through the junction when "the tap is open."

We consider that these two problems are *distinct*, and indeed, the long-standing controversy on tunneling theories arises in part from a failure to identify separately difficulties (i) and (ii). The latter, for instance, is completely avoided if instead of using a *continuous* wave function $\Psi(x)$, one works on a *discrete* tight-binding model, in which the electrons are localized on the sites of a regular lattice. In such a case, the Hamiltonian describes hopping between neighboring sites, say nearest neighbors for simplicity. The division between two distinct halves (sites left or right of some arbitrary boundary) is natural, and the "transfer Hamiltonian" $T$ is unambiguous: hopping across the boundary. Note that the use of such discrete systems does not require any boundary condition; as usual, they are built in the discrete secular equations. Difficulty (ii) thereby never arises.

Yet, problem (i) is still there. Our first paper purported to show how in such a simplified case, one could *exactly* solve the problem by treating the hopping term $T$ to infinite order in perturbation theory, the bias being established at time $t = -\infty$, when the coupling between the electrodes was *strictly* zero (a condition necessary for a finite bias to be consistent with thermodynamic equilibrium). As soon as $T$ is established, the system is off equilibrium, and our contribution was to show how the Kjeldysh formalism allowed to circumvent the assorted difficulties and paradoxes met in earlier theories. This is the key to applying perturbation theory—and indeed Feuchtwang uses that same approach.

Problem (i) being thereby solved, problem (ii) was discussed, and in our opinion solved, in a second paper.[3] There, the continuous function $\Psi(x)$ was constructed as the limit of a "stepped" function when the width of each step goes to zero, namely,

$$\Psi(x) \to \Psi_n \quad \text{if } n\epsilon < x < (n+1)\epsilon \quad (\epsilon \to 0) \,. \tag{1}$$

Such a procedure is familiar in elementary calculus (it is just what one does in order to define Riemann integrals). The derivatives of $\Psi$ appear as limits

$$\Psi'(x) = \lim_{\epsilon \to 0} \frac{\Psi(x+\epsilon) - \Psi(x)}{\epsilon} \,,$$
$$\Psi''(x) = \lim_{\epsilon \to 0} \frac{\Psi(x+\epsilon) + \Psi(x-\epsilon) - 2\Psi(x)}{\epsilon^2} \,. \tag{2}$$

The Schrödinger equation becomes a *difference* equation, which couples $\Psi_n$ to $\Psi_{n\pm1}$. Retaining here only, for simplicity of the argument, the kinetic energy (which allows the electrons to move) this amounts to writing

$$H\Psi_n = -\frac{\hbar^2}{2m\epsilon^2} (\Psi_{n+1} + \Psi_{n-1} - 2\Psi_n). \tag{3}$$

Our formulation is therefore mathematically

*isomorphic* to a tight-binding problem with Hamiltonian

$$H = T(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n - 2c_n^\dagger c_n), \tag{4}$$

$$T = -\hbar^2/2m\epsilon^2 , \tag{5}$$

in which we let $\epsilon \to 0$, $T \to \infty$. That the limit corresponds to free electrons is obvious if one considers the energy spectrum of Bloch waves

$$\epsilon_k = 2T(\cos k\epsilon - 1) \Rightarrow -Tk^2\epsilon^2 = \hbar^2k^2/2m . \tag{6}$$

In this way, the continuous system appears as the *limit* of a discrete system when $\epsilon = 0$. Claiming that such a formulation is limited to tight-binding solids is meaningless; it is precisely designed to describe free electrons. It is tantamount to denying Riemann's limiting procedure for defining integrals. Contrary to what is suggested by Feuchtwang, we never identify $T$ with $p^2/2m$. This is stated explicitly and at length in Ref. 3.

Such a procedure for constructing continuous wavefunctions may be awkward, but at least it is *completely unambiguous*, contrary, again, to what is claimed in Ref. 1. It leads to an explicit expression for the current, which we did prove.

The work of Feuchtwang is based on the use of a different mathematical procedure to relate the properties of the infinite medium to those of two separate halves. We do not question his approach. Indeed, he shows that the mathematical description is not unique; one may choose as a basis for the two *uncoupled* halves a set of wavefunctions with arbitrary boundary conditions at the interface, provided they correspond to a zero current there. For instance, they may correspond to $\Psi = 0$ or $d\Psi/dx = 0$. Feuchtwang essentially shows that a complete set for the whole system is provided by these uncoupled wave functions *and* their derivatives. In our formulation, there was no freedom of boundary conditions, the latter being built in the discrete limiting procedure (when $\epsilon \to 0$, they imply $\Psi = 0$ at the interface). In this respect, Feuchtwang's work provides an extended, albeit equivalent, formulation.

Finally, nowhere did we claim in our continuous-wave-function approach that the tunneling current is proportional to any local density of states [Eq. (40), Ref. 3]. Such densities of states anyhow have no direct physical meaning, as they depend on the arbitrary choice of boundary conditions for the separate electrodes. The result found by Feuchtwang with the choice opposite to ours ($d\Psi/dx = 0$), while definitely simpler formally, does not seem to us physically more transparent.

We hope that these few comments will help to clarify the meaning of our previous papers.

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