Generalized transfer Hamiltonian for the study of resonant tunneling

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Tunneling of electrons through a barrier has been commonly studied by means of a transfer-Hamiltonian method that is not appropriate for describing resonance effects. We generalize that formalism by carrying out an infinite-order time-dependent perturbation theory. Transition probabilities per unit time turn out to be a function of the total Green's function of the system, allowing the study of problems where real intermediate states are involved. We check the method by obtaining excellent results when it is applied to cases in which the exact solution is known.

I. INTRODUCTION

The transfer Hamiltonian (TH) formalism[1,2] is one of the most useful tools for the study of tunneling through barriers separating two semiinfinite media. The idea of that approach is to analyze the total Hamiltonian H of the system by means of a first-order time-dependent perturbation theory applied to the eigenstates of two unperturbed Hamiltonians H_L and H_R describing the left and right sides of the system, respectively. With this procedure, the transition probability from an eigenstate $|L\rangle$ of H_L to an eigenstate $|R\rangle$ of H_R is given by a kind of Fermi's golden rule[2]

$$P_{LR}=\frac{2\pi}{\hbar}\delta(E_L-E_R)\,|\,T_{LR}\,|^2\,, \tag{1}$$

E_L and E_R being the corresponding eigenvalues of H_L and H_R and

$$T_{LR}=\frac{-\hbar^2}{2m^*}\int(\phi_R\nabla\phi_L-\phi_L\nabla\phi_R)\cdot d\mathbf{S}_{LR}\,, \tag{2}$$

with $\phi_L(\mathbf{r})=\langle\mathbf{r}\,|\,L\rangle$ and $\phi_R(\mathbf{r})=\langle\mathbf{r}\,|\,R\rangle$, the current being evaluated on a surface S_{LR} separating the left and right regions. The weaknesses of the method are connected with the fact that it is a first-order perturbation theory. For simple problems, as the tunneling through a square barrier, this reflects only in the lack of an estimation of errors. However, TH becomes unable for describing more interesting problems where real intermediate states are involved.[3-5] One possibility is to extend TH to the case of three spatial regions,[6] but this is only useful for a few simple problems. Therefore, the aim of this paper is to proceed to all orders in perturbation theory to get a formalism in which resonance effects are fully described. On top of standard problems as the double barrier tunneling, the method appears to be especially suitable for cases as magnetotunneling, where a good approximation to the Green's function of the total system can be computed.

In Sec. II we present a time-dependent perturbation theory up to infinite order to describe tunneling processes. We get transition probabilities which are formally different for a continuous spectrum than for a discrete one. The formalism allows the introduction of resonance effects in a very simple way as it is shown in Sec. III. There, we apply this theory to a problem with exact solution to check the capability of the method. Section IV contains a brief summary

II. GENERALIZED TRANSFER HAMILTONIAN

We want to develop a generalized transfer Hamiltonian (GTH) formalism by starting from the same grounds than in the TH but going far beyond. It will require a careful analysis of the time-dependent perturbation theory. For discussion purposes we sketch in Fig. 1 the procedure for a system with a double barrier and an applied bias in the center region, but the method is valid for any other structure. As mentioned above the total Hamiltonian H [Fig. 1(a)] is separated in left and right terms by means of two Hamiltonians $H_L\equiv H$ [Fig. 1(b)] in the left side and $H_R\equiv H$ [Fig. 1(c)] in the right side. We use an interaction picture to switch on adiabatically the required perturbations to recover the total H. So, we write

$$H\equiv H_L+V_L e^{\eta t}=H_R+V_R e^{\eta t}\,. \tag{3}$$

Adiabatic switching means that the process is initiated in $t=-\infty$ and η is going to zero. For perturbative purpose V_L and V_R will be considered of the same order. We start with a time-dependent wave function for the total system

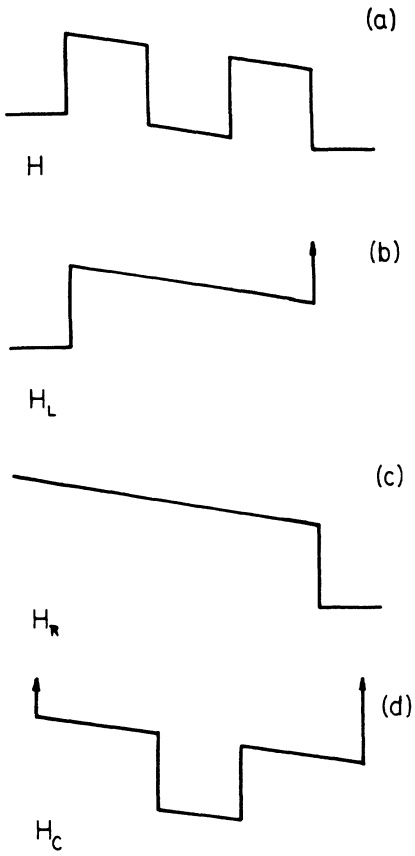

FIG. 1. Sketch of the different Hamiltonians used to study tunneling with the GTH method. (a) Total, (b) left, (c) right, and (d) center Hamiltonians.

$$|\Psi(t)\rangle = f(t)e^{-i\omega_L t}|L\rangle + \sum_R a_R(t)e^{-i\omega_R t}|R\rangle , \tag{4}$$

where $\omega_L = E_L/\hbar$ and $\omega_R = E_R/\hbar$. Tunneling is related to very specific boundary conditions. At the initial time, $|\Psi(-\infty)\rangle$ must describe a particle on the left side. This is fulfilled by imposing

$$f(-\infty)=1 \quad \text{and} \quad a_R(-\infty)=0 . \tag{5}$$

After a while the particle in a precise left state $|L\rangle$ can in principle evolve to any state $|R\rangle$ to the right so that a summation upon R is required in Eq. (4). The time-dependent coefficients are determined from the Schrödinger equation by an expansion in a perturbation series. We take

$$f(t)=f^{(0)} \quad \text{and} \quad a_R(t)=\sum_{j=1}^{\infty} a_R^{(j)}(t) , \tag{6}$$

where the superindices denote the perturbation order. We have made use of the fact that the set $|R\rangle$ is a basis so that no higher orders are required for $f(t)$. The lack of zero order for $a_R(t)$ is a consequence of the boundary conditions. Since we look for density probabilities some care is needed on the normalization of $|\Psi(t)\rangle$. In the Appendix we show that the wave function for any order j is normalized up to this order. With this wave function, the Schrödinger equation gives to first order

$$i\hbar\frac{\partial a_R^{(1)}}{\partial t}|R\rangle = e^{i\omega_{RL}t}e^{\eta t}V_L|L\rangle , \tag{7}$$

where $\omega_{RL}=\omega_R-\omega_L$. For higher-orders one has

$$i\hbar\frac{\partial a_R^{(j)}}{\partial t}|R\rangle = \sum_{R_1} e^{i\omega_{RR_1}t}a_{R_1}^{(j-1)}(t)e^{\eta t}V_R|R_1\rangle . \tag{8}$$

These iterative equations are solved by projecting them on the state $\langle R|$, giving

$$a_R^{(1)}(t)=\frac{1}{i\hbar}\langle R|V_L|L\rangle\int_{-\infty}^{t} dt_1 e^{\eta t_1}e^{i\omega_{RL}t_1} \tag{9}$$

and

$$a_R^{(j)}(t)=\frac{1}{(i\hbar)^j}\sum_{R_1,R_2,\ldots,R_{j-1}}\langle R|V_R|R_1\rangle\langle R_1|V_R|R_2\rangle\cdots\langle R_{j-1}|V_L|L\rangle \times\int_{-\infty}^{t} dt_1 e^{\eta t_1}e^{i\omega_{RR_1}t_1}\int_{-\infty}^{t_1} dt_2 e^{\eta t_2}e^{i\omega_{R_1R_2}t_2}\int\cdots\int_{-\infty}^{t_{j-1}} dt_j e^{\eta t_j}e^{i\omega_{R_{j-1}L}t_j} . \tag{10}$$

The solution is

$$a_R^{(j)}(t)=\sum_{R_1\cdots R_{j-1}}\frac{\langle R|V_R|R_1\rangle\langle R_1|V_R|R_2\rangle\cdots\langle R_{j-1}|V_L|L\rangle e^{i\omega_{RL}t}e^{j\eta t}}{(-\hbar)^j(\omega_{RL}-ij\eta)[\omega_{R_1L}-i(j-1)\eta]\cdots(\omega_{R_{j-1}L}-i\eta)}$$
$$=\frac{e^{i\omega_{RL}t}e^{j\eta t}}{E_L+ij\eta-E_R}\langle R|V_R G_R^{+}[E_L+i(j-1)\eta]V_R\cdots V_R G_R^{+}(E_L+i\eta)V_L|L\rangle , \tag{11}$$

where $G_R^{+}(E_L+i\alpha\eta)$ is the incoming Green's function for H_R commonly used in scattering theory.[7]

Once the wave function $|\Psi(t)\rangle$ is determined to all orders it is possible to calculate the transition probability from left to right per unit time,

$$P_{LR}=\lim_{\eta\to 0}\frac{d}{dt}\,|\,a_R(t)\,|^2\,. \tag{12}$$

Using (6) and (11), Eq. (12) becomes

$$P_{LR}=\lim_{\eta\to 0}\sum_{m,n}\frac{(m+n)\eta e^{(m+n)\eta t}}{(m\eta-iE)(n\eta+iE)}\langle L\,|\,V_L G_R^+[E_L+i(m-1)\eta]V_R\cdots G_R^+(E_L+i\eta)V_R\,|\,R\rangle$$
$$\times\langle R\,|\,V_R G_R^+(E_L+i\eta)\cdots V_R G_R^+[E_L+i(n-1)\eta]V_L\,|\,L\rangle\,, \tag{13}$$

where $E=E_L-E_R$. This equation has to be handled in different ways depending upon whether the spectrum is continuous or discrete. Let us start with the continuous case. Then, there are no divergences in the analytic expression of the Green's functions so that the limit $\eta\to 0$ of the matrix elements can be taken independently from that of the fractions which result to be $(2\pi/\hbar)\delta(E)$ for any m and n. Then, for a continuun the transition probability per unit time is

$$P_{LR}^c=\frac{2\pi}{\hbar}\delta(E_L-E_R)\sum_{m,n}\langle L\,|\,V_L[G_R^+(E_L)V_R]^{m-1}\,|\,R\rangle\langle R\,|\,[V_R G_R^+(E_L)]^{n-1}V_L\,|\,L\rangle$$
$$=\frac{2\pi}{\hbar}\delta(E_L-E_R)\,|\,\langle L\,|\,V_L(I+G_R^+V_R+G_R^+V_R G_R^+V_R+\cdots)\,|\,R\rangle\,|^2$$
$$=\frac{2\pi}{\hbar}\delta(E_L-E_R)\,|\,\langle L\,|\,V_L+V_L G^+V_R\,|\,R\rangle\,|^2\,, \tag{14}$$

I being the unity operator and G^+ the incoming Green's function corresponding to the total Hamiltonian.

We will discuss the implications of Eq. (14) after having the equivalent equation for a system with a discrete spectrum which is more cumbersome. In such a case the limit $\eta\to 0$ implies to have poles in G_R^+ for $E_{R_i}=E_L$ that can coincide with the poles at $E_R=E_L$ for the fractions in Eq. (13). This is a consequence of the fact that the spectral representation of G_R^+ contains the state $|\,R\rangle$. The contributions coming from the poles of G_R^+ can be associated in sets corresponding to $m+n$ constant. For low orders in the perturbation series, i.e., for $m+n=1$, 2, or 3, it is possible to check that the contribution of each set cancels out. In a discrete spectrum the extension of this result to any order allows one to substitute in Eq. (13) the Green's function $G_R^+(E_L)$ by

$$g_R^+(E_L)=\sum_{R_i\neq R}\frac{|\,R_i\rangle\langle R_i\,|}{E_L^+-E_{R_i}}=(I-\mathbb{P}_R)G_R^+(E_L)$$
$$=\mathbb{P}G_R^+(E_L)\,, \tag{15}$$

where $E_L^+=\lim_{\eta\to 0}E_L+i\eta$ and $\mathbb{P}_R$ is the projection operator on the state $|\,R\rangle$, while $\mathbb{P}$ is defined by the last part of Eq. (15). Then, the limit $\eta\to 0$ can be taken in a similar way to the case of a continuous spectrum and the transition probability in the discrete case becomes

$$P_{LR}^D=\frac{2\pi}{\hbar}\delta(E_L-E_R)\,|\,\langle L\,|\,V_L(1+g_R^+V_R+g_R^+V_R g_R^+V_R+\cdots)\,|\,R\rangle\,|^2\,. \tag{16}$$

The series in Eq. (16) is managed in a better way if one considers $\mathbb{P}$ associated to V_R instead of to G_R^+. Then

$$g_R^+V_R+g_R^+V_R g_R^+V_R+\cdots=[G_R^++G_R^+(\mathbb{P}V_R)G_R^++\cdots]\mathbb{P}V_R$$
$$=(E_L^+-H_R-\mathbb{P}V_R)^{-1}\mathbb{P}V_R$$
$$=(E_L^+-H+\mathbb{P}_R V_R)^{-1}\mathbb{P}V_R\,. \tag{17}$$

So, the transition probability is given by

$$P_{LR}^D=\frac{2\pi}{\hbar}\delta(E_L-E_R)\,|\,\langle L\,|\,V_L+V_L G^+(1-\mathbb{P}_R V_R G^+\cdots)\mathbb{P}V_R\,|\,R\rangle\,|^2\,. \tag{18}$$

In many practical cases the parentheses in Eq. (18) can be well approximated by the unity so that P_{LR}^D recovers a shape very similar to P_{LR}^C. The first term $\langle L\,|\,V_L\,|\,R\rangle$ in the matrix elements of P_{LR}^D and P_{LR}^C is the one coming from first-order perturbation and consequently the only one appearing in the TH method. In the simple case of tunneling through a single barrier this is the most important term, the other ones being negligible so that TH is a good approximation. The differences between the expressions for P_{LR}^C and P_{LR}^D are simply a consequence of the

fact that zeros in denominators of the spectral representation of a Green's function must be excluded in the discrete part of the spectrum while they can be kept and integrated in the continuous part of the spectrum.[8]

We want to stress that the expressions we have obtained for the transition probabilities P_{LR}^{C} and P_{LR}^{D} contain explicitly the Green's function of the total system. That means a significant improvement on the TH method because now all the processes involving complicated geometrics[9] or real intermediate states can be fully described. Section III is devoted to see how such a task can be done in a simple and precise way.

III. RESONANCE EFFECTS

The interest of expressions (14) and (18) for the transition probability is the appearance of the total Green's function. In many cases G^+ can be computed but, in general, it is much more appealing to look for approximations to G^+ which contain the main physics of the problem. This is the case of resonance effects that can be easily treated in G^+. In order to discuss these questions we apply the GTH method to the problem of tunneling through a double barrier. In this case, the transmission can be calculated exactly[5,10] so that we can use it as a test for the GTH method. The potential profile is depicted Fig. 1. Resonance effects are due to transitions from left to right by means of virtual processes involving resonance states localized in the well. Therefore the main physics is just connected with well states so that a good approximation is to substitute G^+ by the Green's function G_c^+ of a center Hamiltonian H_c as the one shown in Fig. 1(d). For energies below the barriers this is a very simple approach because only a few localized states are important for the spectral representation of G_c^+. This approximation can be too drastic because it uses discrete δ-functions to describe a continuum with resonant states. It is rather easy to improve the approach in order to recover the continuous aspect of the density of states. We use a self-energy

$$\Sigma = V_c + V_c G_c^+ V_c \ , \tag{19}$$

so that the approximation for G^+ is

$$G^+ \simeq G_c^+ (1 - \Sigma G_c^+)^{-1} \tag{20}$$

which remains very simple to handle. For the case we are concerned with, the wave functions have simple expressions and all the required integrals are analytically performed. In Fig. 2 we show $\ln |T_{LR}|^2$ as a function of the energy $E_L = E_R$, with

$$T_{LR} = -\frac{\hbar^2}{2m^*} \langle L | V_L + V_L G^+ V_R | R \rangle \ . \tag{21}$$

We present the results for the two approximations $G^+ \simeq G_c$ and $G^+ \simeq G_c^+ (1 - \Sigma G_c^+)^{-1}$ as well as the exact result for this transmission[10] in the case of the double barrier shown in the inset and an effective mass of 0.067. Since the three results cannot be distinguished, in the lowest part of the figure we show the error made by taking the above-mentioned approximations. We have performed the same calculation for different values of the parameters having the same behavior for the transmission: for $G^+ \simeq G_c^+$ a small error that is corrected by introducing the self-energy. These results are in support of the GTH method as a simple and efficient tool to study tunneling.

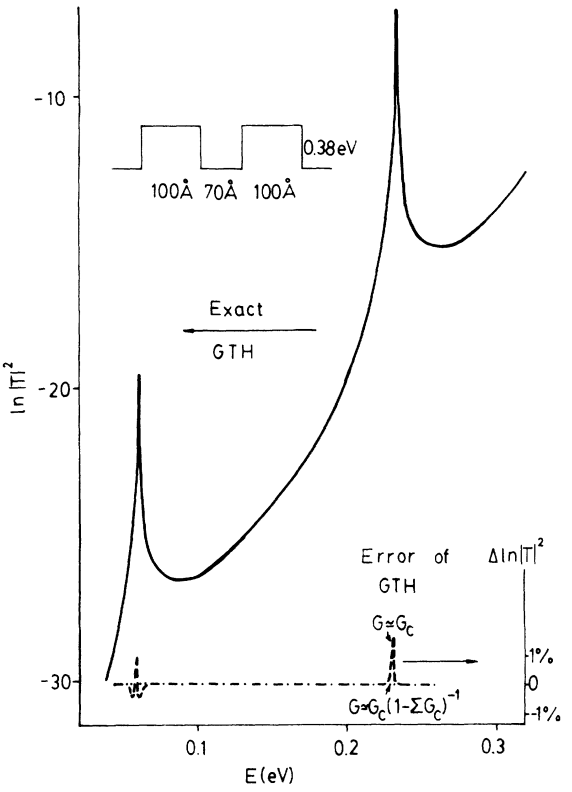

FIG. 2. Logarithm of the transmission coefficient as a function of the energy (in eV) for an electron with $m^* = 0.067$ tunneling through the double barrier shown in the inset. The exact results (Ref. 10) and the ones obtained with GTH are undistinguishable for each other. Lower part of the figure shows the error introduced by GTH by using two different approximations: $G \simeq G_c$ (- - -) and $G \simeq G_c (1 - \Sigma G_c)^{-1}$ (. . .).

IV. SUMMARY

We have extended the TH method to all orders in perturbation theory. This allows the study of tunneling phenomena including resonance effects. The transition probability results to have a different expression for the case of a discrete spectrum than for a continuous one, but in both cases it takes a shape similar to a Fermi's golden rule. The transition probability explicitely depends on the Green's function G of the total system. Resonance effects in double barriers are well described by approximating G by the Green's function G_c of the central well corrected by a self-energy Σ that essentially takes into account the fact that one is working with a continuous spectrum. This formalism is very suitable to introduce

self-consistency connected with the charge density staying at the well. This can be done by means of its effect on G_c and Σ. The formalism is well adapted to treat some other interesting problems. For instance the application of GTH to magnetotunneling with the magnetic field applied either parallel or perpendicular to the current is the subject of a subsequent paper.

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APPENDIX

We want to show that the wave function given by Eqs. (4), (6), and (11) if for any order j normalized up to this order. We start with the case of first order,

$$|\Psi^{(1)}(t)\rangle = f^{(0)} e^{-i\omega_L t}|L\rangle + \sum_R a_R^{(1)}(t) e^{-i\omega_R t}|R\rangle . \tag{A1}$$

Since the normalization to zero order gives $f^{(0)}=1$, we have up to first order

$$\begin{aligned} 1 &= \langle \Psi^{(1)} | \Psi^{(1)} \rangle \\ &= 1 + 2\,\mathrm{Re} \sum_R e^{i\omega_{LR} t} \langle L | R \rangle a_R^{(1)} \end{aligned} \tag{A2}$$

so the last term of the right side must be zero. In order to check this we use the solution (11) for $a_R^{(1)}$ that gives

$$\begin{aligned} &\mathrm{Re} \sum_R a_R^{(1)} e^{i\omega_{LR} t} \langle L | R \rangle \\ &\quad = \mathrm{Re} \sum_R \frac{\langle L | R \rangle \langle R | V_L | L \rangle}{-\hbar(\omega_{LR} - i\eta)} e^{\eta t} \\ &\quad = \mathrm{Re} \langle L | G_R^+(E + i\eta) V_L | L \rangle e^{\eta t} . \end{aligned} \tag{A3}$$

The Green's function of the left Hamiltonian can be written in terms of the one of the right Hamiltonian

$$\begin{aligned} G_R(\omega) &= (\omega - H_R)^{-1} \\ &= (\omega - H_L - V_L + V_R)^{-1} \\ &= G_L(\omega) + G_L(\omega)(V_R - V_L) G_L(\omega) + \cdots . \end{aligned} \tag{A4}$$

The term we are analyzing becomes

$$\begin{aligned} e^{\eta t} [&\mathrm{Re} \langle L | G_L(E_L + i\eta) V_L | L \rangle \\ &+ \mathrm{Re} \langle L | G_L(E_L + i\eta)(V_R - V_L) G_L(E_L + i\eta) V_L | L \rangle \\ &+ \cdots] . \end{aligned} \tag{A5}$$

The terms beyond the first in (A5) are of orders higher than first so that we only need to analyze the first one, which is

$$\begin{aligned} &\mathrm{Re} \langle L | G_L(E_L + i\eta) V_L | L \rangle \\ &\quad = \sum_{L'} \langle L | L' \rangle \langle L' | V_L | L \rangle \frac{E_L - E_{L'}}{(E_L - E_{L'})^2 + \eta^2} = 0 . \end{aligned} \tag{A6}$$

So we have checked that the last term in (A2) is zero to first order which implies $|\Psi^{(1)}(t)\rangle$ is normalized up to first order. It is straightforward to repeat these arguments for any order $|\Psi^{(j)}(t)\rangle$ obtaining the normalization we were looking for.

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