Semiclassical Theory for Dissipative Tunneling towards the Medium

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The exact semiclassical wave function for a tunneling electron, coupled to the degrees of freedom of the host medium, is constructed. In our derivation the tunneling path is divided into an infinite set of infinitezimal segments and the decaying solutions of the stationary Shrödinger equations are matched for each neighboring segment from the beginning to the end of the tunneling path. This solution is expressed as the integral over imaginary tunneling time τ ' (the time of classical motion in the inverted barrier)

$$\Psi_{M}(x(\tau)) = \exp(-S_{0}(\tau))T^{-1}\exp\left\{-\int_{0}^{\tau}d\tau'\hat{V}_{M}(\tau',-i(\tau'-\tau))\right\}\Psi_{M}(x=0),$$

$$\hat{V}_{M}(\tau',t) = \exp(itH_{M})V_{M}(\tau')\exp(-itH_{M}),$$

where H_M is the media Hamiltonian and V_M stands for the interaction of the media with the tunneling particle and S_0 is the classical tunneling action. In partial cases the results of previous analytical studies^{1,2} are reproduced. Our solution covers adiabatic and nonadiabatic tunneling regimes and the crossover between them, when the dissipation reaches maximum.

As a specific application of the result we consider the tunneling of the electron interacting with the optical phonons through the molecular wire. It is shown that the tunneling rate increases due to this interaction that reduces the tunneling barrier, while the effect of dissipation is less significant in agreement with recent numerical studies. Generally one can distinguish three effects of medium on tunneling. The reduction occurs due to the small overlap of initial and final state of the medium and possibly due to the dissipation, while the enhancement results from the reduction of the tunneling barrier due to the reorganization of the medium. Initial and final states of phonons coincide in the case of molecular wire, while the reorganization enhancement is more important as compared to the dissipation suppression.

Calculated current voltage characteristic of the molecular wire shows kinks, when the applied voltage becomes equal to the integer number of phonon quanta in agreement with STM measurements.

Our result can be used to interpret the effect of the medium excitations on tunneling in solids. Interaction of tunneling states in metal glasses with conducting electrons can increase the effective tunneling amplitude because the majority of electrons are fast and contribute to the enhancement. Thus the stronger the interaction, the larger the tunneling amplitude will be. In particular the weak interaction of low energy tunneling systems with the electrons reported in Ref. [3] can be explained by this correlation.

- 1. M. Yu. Sumetskii, Sov. Phys. JETP 62, 355 (1985).
- 2. E. Pazy, B. Laikhtman, Phys. Rev. B 59, 15854 (1999).
- 3. R. König, P. Esquinazi, and B. Neppert, Phys. Rev. B 51, 11424-11432 (1995)