QUANTUM MECHANICAL TUNNELLING IN THIN SOLID JUNCTIONS

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for the award of the degree of
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by

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CERTIFICATE

This is to certify that the dissertation entitled "Quantum Mechanical Tunnelling in Thin Solid Junctions" which is being submitted by Mr. N.S.T. Sai to Indian Institute of Technology, Delhi is a record of bonafide research work carried out by him under my guidance and supervision. He has also pursued the prescribed course of research.

I am satisfied that the thesis presented by him is worthy of consideration for the award of the degree of Doctor of Philosophy. The results contained in it have not been transmitted in part or in full to any University or Institute for any award of degree or diploma.

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N.S.T. Sai

ABSTRACT

When a microscopic particle like an electron negotiates a given region of space where its potential energy exceeds its kinetic counterpart (i.e., a potential barrier) classically it is expected to turn back the moment its velocity tends to be imaginary. But on account of its customary wave nature, it is known to possess a finite probability of escape even across such a barrier when the latter's width happens to be around the de Broglie wave length of the electron. Such a phenomenon has come to be known as Quantum Mechanical Tunnelling.

Conventionally, it has been studied by two distinct approaches namely; time-independent and time-dependent. In the former approach in order that the electron energy must remain the same before and after the process (as thought to be required by the principle of energy conservation) the time-independent Schrodinger wave equations are written and solved in the three regions of space as generated by the barrier and the corresponding wave functions are matched at the appropriate boundaries to evaluate the electron tunnelling probability. The electron tunnelling current density is next obtained by substituting the barrier wave function in the expression for the current density operator and is found to be given by the product of the incident current density and the tunnelling probability. As it is required by the principle

of continuity the above current density also turns out to be identical in the three regions of space. No description of tunnelling time could be possible in this approach, because it rests upon the time-independent principles.

In the early days, such a tunnelling dynamics has been reported to be quite successful in explaining the phenomenon of α -decay, field-emission of electrons from cold metals and so on. But there was difficulty in properly accounting for the finite limit of resolution of the field-emission microscope because the problem demanded a distribution in energy amongst field-emitted electrons against the basic working principle of the theory.

The physics of the effect took an interesting turn with the development of tunnel diode by L. Esaki. He proposed a semi-empirical relation to quantitatively explain the device I-V curve. But this could not be understood on the basis of the above mentioned time-independent approach. But his expression seemed to bring out a new feature of the effect in the dependence of the tunnelling current on the density of states function at the transmitted end. To provide his expression a theoretical basis Bardeen revived the perturbation treatment of tunnelling once proposed by Oppenheimer to explain field-ionization of hydrogen atoms. In this calculation, the transition rate prescribed by the Fermi's Golden rule of the time-dependent perturbation theory has been taken as a measure of the tunnelling current. In spite of all these the physical meaning of the constant 'A' appearing before Esaki's expression could not be understood. Although the phenomenon could then be explained in time-dependent terms, no attempt was made to account for the tunnelling time in a convincing manner. Interestingly enough the predictions of the two theories as regards the magnitude and nature of the tunnelling current density variations were concerned agreed favourably with each other in spite of the fact that these two approaches were essentially independent of one another. However, these current density magnitudes were 10^{-5} to 10^{-6} times smaller as compared to actual experimental values. The theoretical understanding of the tunnel effect became all the more complex with the introduction of Josephson effect as the latter was not easy to be conceived on any of the above formalisms. Several other weaknesses of the theoretical models also become apparent on closer analysis. The case of tunnelling time may be taken as one example. Tunnelling of electrons is indeed a time-dependent event and therefore, a certain time ($\sim \Delta t$) howsoever small it may be, must elapse in its observation. Consequently, the electron energy immediately after the event cannot continue to remain the same as it was before hand but would at least be uncertain by ($\hbar/\Delta t$) as predicted by the Heisenberg's uncertainty principle and this has to be of the order of the barrier height. Since such a spread in its original energy cannot be ignored, the conventional belief of the particle energy remaining the same before and after the process seems untenable. It should be stressed here that this energy uncertainty which has been introduced during the process is neither caused by the use of any faulty apparatus nor due to a particular experimental technique employed to observe the effect. But it has been brought about by the necessary and unavoidable interaction between the electron and the barrier during the process of tunnelling as it is prescribed by the postulates of wave mechanics. Therefore, any denial of the applicability of the principle of uncertainty to the tunnelling problem is equivalent to rejecting the founding postulates of the quantum theory.

Energy distribution of electrons during tunnelling thus becomes a natural and an immediate consequence when the principle of uncertainty is invoked to describe the effect. Roy (1970) was the first to arrive at the Esaki integral on presuming such a distribution. Its physical form was later obtained on the basis of a time-dependent potential function that was regarded to act only during tunnelling. (1977). Such an approach also led to a derivation of an expression for the tunnelling time as well as that of the tunnelling current density for the first time.

But in our earlier derivation there were certain assumptions made as regards the time-dependent coefficients of the barrier wave function were concerned. The derivation as presented in this thesis does not rely on such assumptions but obtains these coefficients ab initio by directly solving the Schrodinger's partial differential equation. The barrier wave function is thereafter constructed by using those coefficients in order to obtain the expressions for the tunnelling probability, the tunnelling time and the tunnelling current density. These expressions have next been compared with our earlier results which were originally derived for larger barriers only.

The tunnelling theory so developed is thereafter employed to study the Josephson effect. The direction of the dc Josephson current flow may easily be predicted on the basis of this analysis. An expression for the peak value of Josephson tunnelling current density has also been derived in terms of the barrier and superconducting parameters to explicitly show its temperature dependence. Next a formalism has been developed to study the quasiparticle tunnelling in superconducting junctions on the basis of the new theoretical formulation of tunnelling mentioned earlier. This has next been employed to obtain static tunnelling J-V relations across the said junctions.

During quantum mechanical tunnelling an electron may also lose a part of its energy by exciting atomic or molecular vibrations within the barrier. Such an inelastic process is known to provide an additional path or channel for the tunneling current. To analyse such a process, the tunnelling electron is presumed to acquire an additional component of potential energy due to molecular excitations. The problem is thereafter treated similar to direct tunnelling case in order to obtain the various indirect tunnelling parameters.

In the end bhe results of the thesis have been summarised and compared with the contemporary work, Possible future lines of investigation in this direction have also been suggested.

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