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THE IMPACT PARAMETER DEPENDENCE OF SWIFT ELECTRON-MATTER INTERACTIONS

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(1.0) INTRODUCTION

In quantal collision theories, momentum and energy are usually taken to be good quantal variables. Classical collision theory, on the other hand, uses position and time to describe interactions between a probe and a target. In modern physics one may wish to express quantal theories in terms of spacelike variables. For example, experiments are now common in which one measures, by means of a narrowly focused beam of swift electrons, the distribution in energy of losses experienced in a very small region of space. Also, in experiments with channeled ions, and in microdosimetry, one is interested in the spatial coherence of unlocalized excitations created by swift ions and electrons, and their ultimate localization through transfer of energy to, e. g., single-particle excitations. In this lecture I will describe work, done in part in collaboration with Professor Howie, on some aspects of the spatial dependence of inelastic interactions between a charged particle and a condensed matter target.

(2.1) QUANTAL ASPECTS OF THE SPATIAL RESOLUTION OF ENERGY LOSS MEASUREMENTS IN ELECTRON MICROSCOPY

Aspects of spatial resolution in combined energy-loss-electron microscopy have been considered. Working in the first Born approximation, we have shown[1] that for coherent broad-beam irradiation, the probability of stimulating a localized excitation in matter may be calculated as if the electron were executing classical rectilinear motion, over all impact parameters, at constant velocity, v, as v becomes large compared with $(2E/m)^{1/2}$. Here E is the excitation energy of the target and m is the electron mass. Implicit in this result is the assumption that all inelastically scattered electrons are collected by the spectrometer. Corrections to this recipe are expressed as a power series in inverse powers of v and originate in the quantal properties of the electron. The first correction term has been evaluated explicitly and the resulting impact parameter dependence of the excitation probability has been evaluated numerically for some model systems.

(3.1) INELASTIC SCATTERING PROBABILITIES IN SCANNING TUNNELING ELECTRON MICROSCOPY

A general theoretical expression has been found that describes the probability for collection and energy analysis of inelastically scattered electrons in a scanning transmission electron microscope configuration.[2] It is couched in terms of certain integrals over the matrix element of the density operator with respect to the eigenstates of the target. We have shown that, if all inelastically scattered electrons are collected, then the fraction of incident electrons that will be determined to have given rise to excitation in a localized target at impact parameter b may be calculated by simply convoluting over b, (a) the probability, P_c (b), that a classical electron with the same velocity will create the excitation at the given b, with (2), the probability of finding the electron in the microprobe at that same value of b. We have also shown that even in the opposite extreme, when a small solid angle of axial collection is employed, the energy loss spectrum will still approximate to the classical expression provided that it is normalized to the same loss intensity and if the Fourier-transformed profile function does not become too small for some ranges of its argument. A realistic microprobe distribution has been used to compute the angular distribution of electrons that have created a surface plasmon or a surface optical phonon at a surface parallel to the electron trajectory. These results demonstrate the usefulness of the classical theory for axial detector positions as well as the possibility of enhanced spatial resolution for off-axis detector positions.

(4.1) THE SPATIAL DISTRIBUTION OF COHERENT EXCITATION GENERATED IN CONDENSED MATTER BY SWIFT IONS

As indicated above, other questions, involving the spatial representation of energy transfers in condensed media by swift ions, arise in microdosimetry and other parts of the field of radiation physics. Of considerable interest is the process of localization of initially unlocalized excitations such as plasmons in condensed media[3].

We have considered three alternatives in extracting a spatial representation from the quantal expression of the probability of energy transfer to a condensed medium from a swift charged particle. In the present case one is interested in establishing the impact parameter representation of energy transfer when a heavy ion traverses an extended condensed medium.

(4.2) The Chang-Raman Transformation

In the context of theoretical high energy physics, Chang and Raman[4] have employed a mathematical transformation from momentum to a space-like variable that Fano[5] has advocated for use in radiation physics. For simplicity, we consider the Chang-Raman transform applied to the expression for the probability of plasmon creation in a free electron gas as it depends on momentum transfer from a heavy ion with charge Ze, moving with uniform rectilinear velocity $\underset{\sim}{v}$ in the electron gas. One finds, for b large enough

$$d^2\Lambda^{-1}/db^2 = \frac{Z^2e^2\omega_p}{2\pi\hbar v^2} \exp(-2\omega_p b/v)/b^2 \qquad (1.1)$$

for the differential inverse mean free path for finding the plasmon at impact parameter b relative to the ion path in the interval db^2. The plasmon energy is $\hbar\omega_p$.

(4.3) The Energy-Loss Transform

We have made a more general approach[6] to the problem of finding an impact parameter representation for an ion traveling in a medium characterized by the general dielectric function $\epsilon_{k,\omega}$. Employing a transform different from, but related to, that of Chang and Raman, we find

$$\frac{d^3\Lambda^{-1}}{d\omega d^2b} = \frac{Z^2e^2\omega}{\pi^2\hbar v^3} \int \frac{d^2\kappa}{\kappa^2+\omega^2/v^2} \, I_m\left[\frac{-1}{\epsilon_{k,\omega}}\right]$$

$$\times \left[\frac{\omega}{v} K_o\left[\frac{\omega b}{v}\right] J_o(\kappa b) + \kappa K_1\left[\frac{b\omega}{v}\right] J_1(\kappa b)\right] \qquad (1.2)$$

where the differential inverse mean free path is now differential in ω, the frequency variable.

(4.4) The Impact-Parameter Dependence of Localized Single-Particle Transitions Induced by Unlocalized Excitations

A schematic representation of the spatial dependence of the localization of an initially unlocalized coherent excitation in an extended medium may be found in a straightforward manner. Assume that an impurity site in the medium may be characterized by an electronic orbital $u_o(\underset{\sim}{r})$ located at impact parameter b relative to the path of a swift ion. For simplicity represent the excited states of this electron by orthogonalized plane waves $u_{\underset{\sim}{p}}(\underset{\sim}{r}) = \langle r|k\rangle - \langle \underset{\sim}{k}|o\rangle\, u_o\, (\underset{\sim}{r})$, where $\langle r|k\rangle = \exp(i\underset{\sim}{k}\cdot\underset{\sim}{r})/\Omega$ and Ω is the normalization volume. Ordinary first-order perturbation theory yields the following expression for the impact parameter dependence of the excitation probability,

$$P = \frac{1}{\hbar^2}\sum_{\underset{\sim}{p}} \left| \int_{-\infty}^{\infty} dt\exp(i\omega_{po}t)\ \langle \underset{\sim}{p}|V(\underset{\sim}{r},t)|o\rangle \right|^2$$

where $V(\underset{\sim}{r},t)$ is the potential at the electron in question due to the passing ion. As in Lecture II above, $V(\underset{\sim}{r},t)$ may be expressed simply in terms of the dielectric response function $\epsilon_{k,\omega}$ of the medium. Carrying out this procedure and focusing on the part of the medium response corresponding to coherent, plasmon-type excitations, one finds that the impact parameter dependent of the deexcitation probability resembles more closely that predicted by Eq. (1.2) than that obtained from Eq. (1). In particular, the decrease in p with increasing b is appreciably slower than that displayed in Eq. (1.1).

Figure (1) compares the impact parameter dependence of the energy density per unit impact parameter, multiplied by b^2v^2/Z^2, obtained using the Chang-Raman-Fano transform with that using our energy transfer transform. The calculations were done for 10 MeV protons traversing a free electron gas with ω_p = .5 a.u. Also shown is an estimate of the incoherent energy deposition from delta rays generated by the fast ion. One sees that the result found from the Chang-Raman-Fano method is considerably smaller than that from our approach, especially at large impact parameters. A detailed description of these results is given in Ref. 6.

(5.1) Summary

In this lecture I have sketched some features of the impact parameter dependence of the probability of exciting elementary excitations by swift charged particles. Much remains to be done in this area, particularly with respect to applications of the self-energy approach described briefly in my second lecture.

(6.0) Acknowledgements

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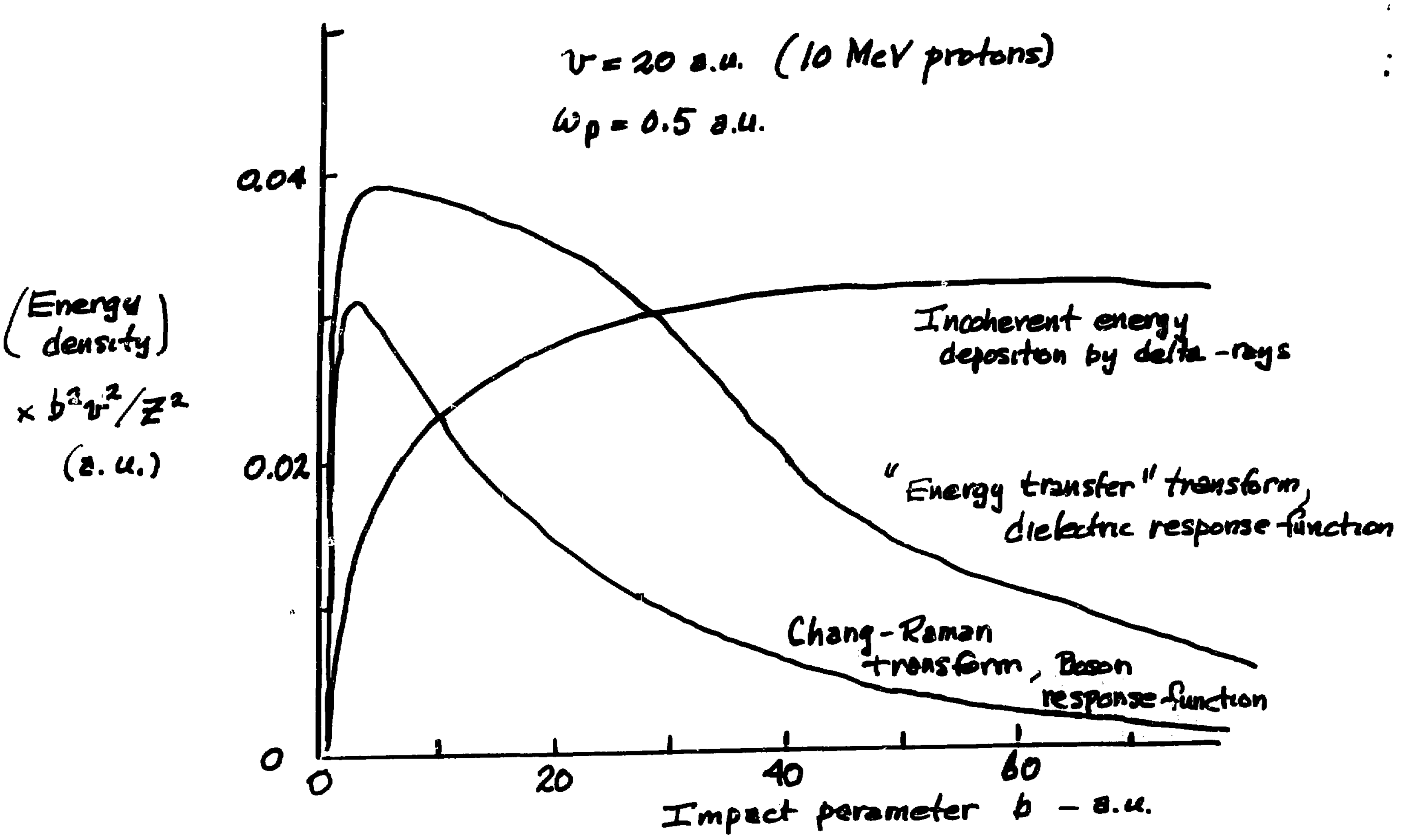

Figure 1. The impact parameter dependence of the energy deposited per unit impact parameter interval due to 10 MeV protons in an electron gas. The curves labeled "Chang-Raman transform" and "Energy transfer transform" correspond to coherent energy transfer. The third curve shows an estimate of energy deposition due to delta rays.