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Quantum Mechanics and Nonadiabaticity in Charged Particle Dynamics in a Magnetic Field

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Abstract

Nonadiabaticity in charged particle dynamics in a magnetic field is explored from the quantum mechanical angle. It is pointed out that a quantum transition is essentially a nonadiabatic process. It is further pointed out that a quantum mechanical entity relating to a transition, namely a "transition amplitude" or more precisely a "transition kernel" in the corresponding limit plays a seminal role in describing quantumnonadiabticity. A set of novel manifestations of the behaviour of the transition amplitude are described which include one-dimensional macroscopic matter wave inteference effects, matter wave beats, and the observation of curl-free vector potential in the macrodomain in one dimension.

I. INTRODUCTION

Nonadiabaticity is understood as a violation of adiabaticity and though adiabaticity has been well described in most books on classical mechanics, the issue of nonadiabaticity had not been addressed adequately until rather recently. It was, however, inherent in the formulation of the Bohr atom the quantization of the adiabatic action invariant. The action was conserved (the adiabatic invariant) so long as the electron remained in a given orbit. Any jump from one orbit to another in a transition signified nonadiabaticity since it changed the action by a finite discrete amount. Thus quantum transitions signified nonadiabaticity.

Of course, a transition is induced by a perturbation. In an atom, a radiation field of a given frequency (acting as a perturbation) would induce transition between two atomic levels à la the time dependent perturbation theory, if the energy of the radiation quantum matches with the energy difference of the two levels. This is the case of the resonance denominator in perturbation theory where the transition probability increases linearly with time, signifying again a change in the action of the system (nonadiabaticity) as a consequence of the perturbation.

In classical charged particle dynamics in a magnetic field when one talks of nonadiabaticity, one refers to changes in an adiabatic invariant when the magnetic field, in which the particle is moving, does not vary (in space and/or in time) slowly enough for the adiabaticity condition to be satisfied. How does this problem translate in terms of quantum mechanics and what new perspectives and results we obtain from such an examination is what I am going to discuss in this talk.

In the course of the present discussion we shall have occasion to point out that nona-diabatic effects are to adiabatic motion what quantum effects are to classical dynamics. However, we shall go a step further, (in fact, a major step further) and show that some of the non-adiabatic effects in charged particle dynamics which manifest in macroscopic dimensions, are in fact real quantum effects and not just quantum-like. This will be seen to be rather novel, not hitherto encountered in the recent half a century of the of the studies of charged particle dynamics. We shall show that these quantum effects do not belong to the micro-domain, as one would normally expect quantum effect to, but rather they manifest themselves in the macro-domain in contradistinction to the normally held belief. The novelty of the results arises because of the latter fact, and in a general sense they are a manifestation of nonadiability.

II. CHARGED PARTICLE DYNAMICS IN QUANTUM MECHANICS

Quantum mechanically a charged particle in a magnetic field is described by Landau wave functions for the dynamics normal to the magnetic field and plane waves for the dynamics along the magnetic field if the magnetic field is uniform. The complete wave function is given by

$$\phi_{N,k} = H_N(x)e^{ikz} \tag{1}$$

where N denotes the Landau quantum number, k, the wave number for the plane wave part and $H_N(x)$ is the harmonic oscillator wave function for the N^{th} Landau state.

$$H_N(x) = e^{-\frac{1}{2}\frac{eB}{\hbar c}x^2} \quad H_N\left(x\sqrt{\frac{eB}{\hbar c}}\right)$$
 (2)

 H_N being the Hermite polynomial, and x, the coordinate normal to the magnetic field and the direction of symmetry.

Consider that a particle is in a given Landau state N and assume that the magnetic field that the particle moves in changes in time, either explicitly or through the particle's motion along the field as the latter varies spatially from point to point. If the change in the magnetic field is slow enough such that $dB/B\Omega dt \ll 1$, or $v_{\parallel}dB/\Omega Bdz \ll 1$, then the particle will, to a high degree of approximation, remain in its initial Landau state. This statement is the quantum analogue of the classical "adiabatic invariance" of the gyroaction $\mu = \mathcal{E}_{perp}/\Omega$, (where \mathcal{E}_{\perp} is the energy in the perpendicular component, and $\Omega = eB/mc$ is the gyro-frequency), which is essentially $\mu = N\hbar$.

There is, however, an important difference between the quantum mechanical and classical statements. Quantum mechanically one would say that the probability amplitude for the particle to remain in its initial Landau state N, would be large, and larger, the smaller the adiabaticity parameter ϵ . Classically, since there is no concept of probability amplitude, associated with a single particle, the gyro-action of the particle at the end of an operation is a definite quantity to be evaluated classically. It turns out that the change in the adiabatic

action invariant $\Delta \mu$ is found to be exponentially small $\sim e^{-1/\epsilon}$, (ϵ being the adiabaticity parameter).

But quantum description imparts a much richer structure to the content of nonadiabaticity. The change in the magnetic field (which amounts to a perturbation) would induce a transition from the initial Landau state N to $N \pm n$ (n > 1). The nonadiabaticity is then specified quantum mechanically, through the probability amplitudes $\Phi(N,n)$ for transition across $n = 1, 2, 3 \dots$ Landau level intervals from the initial Landau level N. Thus while classically there is just one quantity $\Delta \mu$ (number) to describe nonadiabaticity, quantum mechanically there is a set $\{n\}$, of numbers specifying the n amplitudes $\Psi(N,N+n)$. However, Dykhe and Chaplik [1] who were the first to address the problem of nonadiabaticity quantum mechanically, (as a scattering problem) actually identified the n = 1, quantum mechanical nonadiabaticity with the classical nonadiabatic change, through appropriate expectation value.

III. QUANTUM MANIFESTATIONS IN THE MACRO-DOMAIN

The question that we would like to pose here is: Can these quantum non-adiabatic transition amplitudes $\Psi(N, N \pm n)$, n = 1, 2, 3 have physically observable manifestations? We shall point out in what follows that not only do they have physically observable effects but they actually manifest themselves in the macro-domain usually regarded as the preserve of classical mechanics.

A. Nonadiabatic charged particle loss from adiabatic traps

The first such manifestation came in the form of the observation of a multiplicity of residence times in an adiabatic trap against nonadiabatic loss. This was established in

a series of experimental papers by Bora et al. [2], while the experimentation itself was motivated by some unusual productions in a theoretical paper by the author [3].

There is a rather interesting developmental history to these findings. The theory [3] referred to above which motivated these experiments and whose predictions were thus verified, was not a theory in the conventional sense. It was a rather intuitive heuristic construct which yielded a set of Schrödinger-like equations

$$\frac{i\mu}{n}\frac{\partial\Psi(n)}{\partial t} = -\left(\frac{\mu}{n}\right)^2 \frac{1}{2m}\frac{\partial^2\Psi(n)}{\partial z^2} + \mu\Omega\Psi(n) , \quad n = 1, 2, 3,$$
 (3)

with μ being the initial value of the gyroaction, Quantum mechanically $\mu = N\hbar$, with $N \gg 1$. The $\Psi(n)$ in Eq. (1) are essentially the transition amplitude $\Psi(n,N)$ as defined above where N [which represents the initial Landau level and represented by μ in (1)] stands suppressed.

It was not clear then (in 1971, when those equations were delivered) that these were essentially quantum mechanical transition amplitudes. This connection could be established only recently [4] by the author. We shall come to its greater details later. If we do identify the index n in these equation as the Landau level interval (as established in [4]) then the different equations labelled by the indices n = 1, 2, 3, etc. would make different predictions as determined by the value of n.

The main prediction of this set of equations relates to the residence times of charged particles in an adiabatic trap against nonadiabatic loss. Note that $(\mu\Omega)$ occurring in the Schrödinger-like equation (3) as a "potential" is actually the "adiabatic potential" appearing in the adiabatic equation of motion

$$m\frac{dv_z}{dt} = -\frac{\partial}{\partial z} \left(\mu\Omega\right) \tag{4}$$

As is well known, according to this equation a particle will be trapped adiabatically in a potential well, defined by $(\mu\Omega)$ provided the total energy of the particle is $\mathcal{E} < (\mu\Omega)_{max}$, the maximum of the adiabatic potential. There exists a relationship between Eq. (3) and Eq.

(4) in that, in the limit $(\mu/n) \to 0$, Eq. (3) yields the adiabatic equation of motion (4), in the same manner in which the Schrödinger equation yields the classical equation of motion in the limit $\hbar \to 0$.

Thus the Schrödinger-like equation (3) would describe the nonadiabatic leakage as if a "tunnelling" of the adiabatic potential hump, analogously to the quantum tunnelling of the classical potential. Thus given the form of the potential $\mu\Omega$ (or basically the magnetic field variation along the particular line of force on which the particle is) one can calculate from Eq. (3) à la quantum mechanics, the probability of escape across the potential hump from the adiabatically trapping region. The residence time is then the inverse of this probability.

It may be noted that the different equations of the set have the index n, appear in the combination (μ/n) , and will lead to distinct expressions for the residence times depending on n, which are found to be of the form

$$\tau_n \sim \exp\left[n\beta(\mathcal{E}, \delta, L)\right]$$
 (5)

where $\beta(\mathcal{E}, \theta, L)$ is a function of the total energy \mathcal{E} , the pitch angle of injection δ and the characteristic length of the magnetic field variation L, and has the form

$$\beta = \left(\frac{2}{m}\right)^{1/2} \frac{2\pi L e}{c\sqrt{\mathcal{E}}} \left\{ \left(\frac{B_{max} - B_o}{B_{in}}\right)^{1/2} \sin \delta - \left(1 - \sin^2 \delta \frac{B_o}{B_{in}}\right)^{1/2} \right\}$$
 (6)

for the magnetic field variation of the form

$$B = B_o + (B_{max} - B_o) \left(\cosh \frac{z}{L} \right)^{-2} \tag{7}$$

 B_{in} is the value of magnetic field at the point of injection. The most interesting aspect of the expression (5) for the residence time is its dependence on the index n, which is exponential in n.

If we recall the identification of the index n, as pointed out earlier, namely that it corresponds to the Landau level interval across which the probability amplitude $\Psi(n)$ describes the transition amplitude, then the multiplicity of residence times τ_n as described by the

expression (5) constitute a manifestation of a quantum property of the system, since the Landau level interval n is outside the purview of the classical charged particle dynamics. What is fascinating to note is that this multiplicity of residence times have indeed been observed and firmly established through a series of experiments by Bora et al. [2]. Fig. 1 shows $ln\tau_n$ vs. B plots for the multiple residence times corresponding to n = 1, 2. The plots clearly show the slopes to be in the ratio 1:2 as required by Eqs. (5, 6). And what is even more remarkable that these quantum manifestations have appeared in systems with classically macroscopic spatial dimensions.

B. Probability waves in macroscopic dimensions

The next fascinating object that we wish to discuss in this connection following from the above formalism, is the existence of "probability waves" in the macroscopic domain which are described by the transition amplitude governed by Eq. (3).

It is most instructive to look at the quantum mechanical meaning of the wave amplitude $\Psi(n)$ to understand the nature of the macroscopic "probability wave" described by it. As mentioned earlier the $\Psi(n)$ represent the "transition amplitude" generated as a consequence of scattering.

Assume that the scattering of the particle in the state (N, k), [N] representing the Landau quantum number, and k the wave number of the plane wave along the magnetic field direction leads to the new state (N', k') after the scattering. Then the "transition amplitude" for this scattering including the plain wave part, is given by

$$\Phi_{N'N,k'k}^{(z)} = \int dx \phi_{N'k'}^* V(x) \phi_{Nk} = e^{-i(k'-k)z} \int dx H_N'(x) V(x) H_N(x) = e^{-i(k'-k)z} \alpha_{N'N}$$
 (8)

where k' is not a given number, but will be determined from N' and N using energy conservation and $\alpha_{N'N}$ is a number denoting transition amplitude from $N \to N'$ induced by

the perturbation V(x). Note that $e^{-i(k'k)z}$ represents a plane wave (- a transition amplitude wave) with the wave number (k'-k) which, being a difference, can be a very small quantity. Indeed using total energy conservation before and after scattering, we have

$$\frac{(\hbar k')^2}{2m} + (N'\hbar\Omega) = \frac{(\hbar k)^2}{2m} + N\hbar\Omega \quad , \tag{9}$$

where

$$(k'-k) \cong \frac{(N-N')\Omega}{\hbar k/m} = -\frac{n\Omega}{v} . \tag{10}$$

where $v = \hbar k/m$ is the velocity of the particle along z, and we have assumed that (k'-k) is small compared to k, so that $(k+k') \approx 2k$ and n=1, 2, 3,... and $N \gg n$. In fact for typical laboratory conditions, $N \approx 10^8$. Using (10) in (8), we get

$$\Phi_{N'N}(k'-k) = \alpha_{N'N} e^{\frac{in\Omega z}{v}} \tag{11}$$

which represents a plane wave with the wave length

$$\lambda_n = \frac{2\pi v}{n\Omega} \tag{12}$$

For typical laboratory conditons, $\mathcal{E} \approx 1 \text{ keV}$, B = 100 g, $\lambda_1 \approx 4 \text{ cm}$.

1. One-dimensional interference effects observed

One thus predicts the existence of a macroscopic probability matter wave with a wave length ~ 4 cm (for the parameters $\mathcal{E} \approx 1$ keV, $B \approx 100$ g), which predicts resulting matter wave interference effects with such a large wave length. These effects have indeed been observed by Varma, Punithavelu and Varma [5]. Fig. 2 shows the electron current collected by a [collector] plate as the cathode voltage of an electron gun is swept while the electrons from the gun travel along a magnetic field in a vacuum chamber. Sweeping cathode voltage

implies, of course, sweeping the electron energy. If we were to use the classical Lorentz equation to understand the dynamics with the sweeping of the electron energy, one would expect at best a monotonically increasing electron plate current.

However, Fig. 2 shows instead a number of sharp peaks and dips at specific energy values. This curve of Fig. 2 replotted as a function of $\mathcal{E}^{-1/2}$ is shown in Fig. 3. It exhibits the different peaks at equal intervals on the $\mathcal{E}^{-1/2}$ scale.

These peaks are found to fit the relation (which implies that there are integral number of wave length λ_1 in the distance L)

$$L = \ell \,\lambda_1 = \frac{2\pi\ell}{\Omega} (2\pi\varepsilon/m)^{1/2} ,$$

or

$$\Omega L = \frac{2\pi\ell}{\Omega} \left(\frac{2\varepsilon}{m}\right)^{1/2} , \ell = 1, 2, 3, \dots$$
 (13)

for various ℓ values where L is the gun-plate distance. More precisely L is the distance between the anode of the electron gun (where the non-adiabatic transition to another Landau level occurs because of the perpendicular electric field) and the plate. For $\mathcal{E} = 500$ eV, B = 135 g for this curve of Fig. 2, $\lambda \approx 3.7$ cm. Eq. (13) essentially describes the condition for one-dimensional interference effect: namely that L is equal to integral multiple ℓ of the wavelength λ_1 . That the peaks fits the relation (13) demonstrates the existence of macroscopic matter waves of wave length $\lambda = 2\pi v/\Omega = 3.7$ cm.

The wave algorithm which describes these interference effects is as follows:

The primary electron wave emanating the gun-cathode is scattered in the region between the cathode and anode region by the perpendicular component of the accelerating electric field leading to the generation of a "transition amplitude wave" of wave number $k = n\Omega/v$, originating at some point z_o in the region. Then the wave function for this wave at an arbitrary point z is

$$\psi_1(z) = A e^{ik(z-z_o)} , \quad k = n\Omega/v , \quad z > z_o$$
 (14)

Next, as the amplitude of the unscattered wave propagates forward, it comes across a grid located at z_g very close to the collecting plate. The electron wave (the primary unscattered part) thus gets scattered by the grid wires leading to a non-adiabatic transition to another Landau level and generating again the "transition amplitude wave" of wave number $k = n\Omega/v$, originating at $z = z_g$. Then the wave function of this wave propagating $z = z_g$ onwards is

$$\psi_2(z) = A' e^{ik(z-z_g)} , z > z_g$$
 (15)

As these waves reach the plate at $z = z_p$, the total wave amplitude at the plate is

$$\psi_p(z_p) = \psi_1(z_p) + \psi_2(z_p) = A e^{ik(z_p - z_o)} + A' e^{ik(z_p - z_g)}$$
(16)

Taking $|\psi_p(z_p)|^2$, we get (assuming $A \approx a'$)

$$|\psi_p(z_p)|^2 = 2|A|^2 + 2A^*A\cos[k(z_q - z_q)].$$

$$\approx 2|A|^2 \left(1 + \cos\left[k(z_p - z_o)\right]\right)$$
 (17)

if z_g is very close to z_p . The Cosine term in (17) represents the interference term, and since we identify L in (13) with (z_p-z_o) , this term describes the interference maxima through

$$kL = 2\pi\ell$$
 , $\ell = 1, 2, \cdots$

or

$$\frac{\Omega}{2\pi v}L = 2\pi\ell \,\,,\,\, \text{(takingonlyn} = 1) \tag{18}$$

This relation is identical with the relation (13) which fits the observed peaks in Fig. 3.

Two remarks are in order: First, the relation (18) has been written for n = 1, and compared with the relation (13) fitting the observed peaks. n = 2, 3 etc. would correspond to the presence of 2nd and 3rd etc. harmonies. One should expect that these too ought to be observed. The existence of the various harmonies are indeed implied in the sharpness of the observed peaks. The second relates to the necessity of the grid, in the above experiment which is assumed to be close to the plate. In fact, one would still observe the above peaks even if no grid is present. In that case, the surface of the collector plate itself plays the role of the scatterer, while the interior of the plate serves as the collector where the interference effects are detected.

2. "Beats" observed in one-dimensional interference

The experiments that was carried out for the observation of one-dimensional interference effects was extended somewhat, so that we also observed beats. The extension consisted in moving the grid away from the plate over various distances and sweeping the cathode voltage as before. When the grid is at a finite distance away from the plate, this distance plays a distinct role in the dynamics of interference in this case. There are now two distances involved in the process: (i) the gun-plate distance $L_p = z_p - z_o$, and (ii) gun-grid distance $L_g = z_g - z_o$, which act like two different "frequencies" as the wave number k is swept through the sweeping of the electron energy (cathode voltage).

The superpositon of these two waves with the different frequencies L_p and L_g , with $L_p - L_g << L_p$, would lead to the generation of beats. Indeed Fig. 3 does exhibit the existence of such beats. Here the two distance are: $L_p = 51$ cm, and $L_g = 45$ cm, so that $L_p - L_g = 6$ cm. The location of the maxima of the observed beats, have indeed been found to correspond to the difference of frequencies $D = L_p - L_g = 6$ cm, fitting the relation

$$\Omega(L_p - L_g) = 2\pi \ell v \quad , \quad \ell = 1, 2 \cdots$$
 (19)

IV. SCHRÖDINGER-LIKE EQUATIONS FOR THE TRANSITION AMPLITUDE AND OBSERVATION OF CURL-FREE VECTOR POTENTIAL IN THE MACRO-DOMAIN

The Schrödinger-like equations (3) which were first obtained by the author [3] heuristically in 1971 were derived later in 2001 [4] using quantum mechanics in the pathintegral representation. These equations were derived for the "transition amplitudes" for transitions across Landau level intervals n from the initial large Landau quantum state $N \gg 1$, $(N \gg n > 1)$. It was only through this derivation that the identity of the wave amplitudes of Ref. [3] could be established as being the "transition amplitudes". Whereas the equations obtained in Ref. [4] were one-dimensional along the magnetic field, the full three-dimensional equations were obtained in the review [5].

Since they were obtained from quantum mechanics in Ref. [4] and [5], it was possible to include a curl-free vector potential in the derivation. The resulting equations as obtained in Ref. [4] are given by:

$$\frac{i\mu}{n}\frac{\partial\Psi(n)}{\partial t} = \frac{1}{2m}\left(\frac{\mu}{ni}\frac{\partial}{\partial z} - \frac{e}{c}A_z\right)^2\Psi(n) + (\mu\Omega)\Psi(n)$$
(20)

with the total transition probability density given by

$$\rho(z,t) = \sum_{n} \Psi^*(n)\Psi(n) \quad , \tag{21}$$

 A_z in Eq. (20) is the z-component of curl-free vector potential present in the system.

In addition to what has been already described in Sec. III, the presence of A_z in (20) leads to a rather fascinating prediction. It follows from (20) as shown in [5, 6] and with greater clarification in [7], that one can detect the presence of a curl-free vector potential a l à Aharonov-Bohm in macroscopic dimensions, and in fact, in one-dimension rather than two or three. Both these features are contrary to the standard quantum Aharonov-Bohm effect which occurs in the macro-domain, and is usually regarded as of topological origin, and thus occurring in a multiply connected domain.

The experiment to check the observability of the curl-free vector potential [as predicted by Eq. (20)] is performed with a similar arrangement as in the experiment described in Sec. III, but now a curl-free vector potential is produced by inserting a toroid which is wound short way around its closed circular axis, in the path of the electron beam normal to the magnetic field between the gun and the detector. A current in the wires so wound would produce a confined magnetic flux within the toroid, which in turn produces a curl-free vector potential in the space around.

The experiment is performed [6] by first tuning the magnetic field (for a given gun-grid distance L, and the electron energy \mathcal{E} such that the detector current shows a maximum. At this point, the current in the toroid is varied resulting in the variation of vector potential. If the detector current would show no variation with the variation in the toroid current then clearly the vector potential would have no effect on the electron dynamics. However, the experiment does show an oscillatory variation in the detector current as demonstrated in Fig. 4. This exhibits without doubt an effect of the curl-free vector potential on the electron dynamics.

This effect is highly enigmatic on two counts. One, that it is found to manifest in the macro-domain of tens of centimeters. This is, in fact, quite astonishing and enigmatic, since looked at perfunctorily, it would appear to be contrary to the Lorentz equation which does not recognize a curl-free vector potential.

The interesting fact of the matter, however, is that this effect has a quantum origin which manifests itself in the macro-domain. This is esentially the property of transition amplitude $\Psi(n)$ whose evolution is governed by Eq. (20). This may also be the domain of classical dynamics but the effect described here is quantum mechanical. Such a quantum manifestation has not been observed and reported so far. These are entirely new effects. The exact manner of prediction of this effect following from Eq. (20) has been presented in Ref. [8], along with the detailed comparison with the experimental observations.

A final comment ought to be made to clarify the nature of the observed and to pre-empt a possible misunderstanding. It needs to be emphasized that the "transition amplitude" waves which are involved in the effects observed don't exist a priori, but are generated at the points of scattering episodes, and the path lengths are reckoned only from the points of generation. The physical importance of the transition amplitudes and their role in the prediction and description of these phenomena is entirely new and has not been revealed earlier to the best of author's knowledge.

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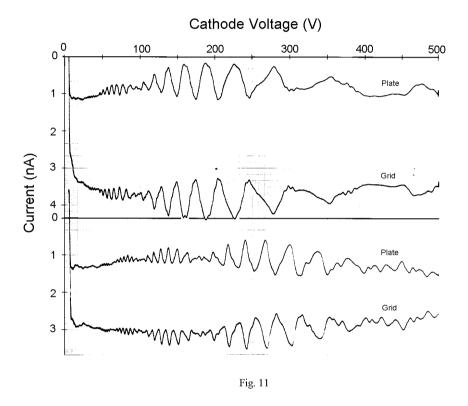


Fig. 2

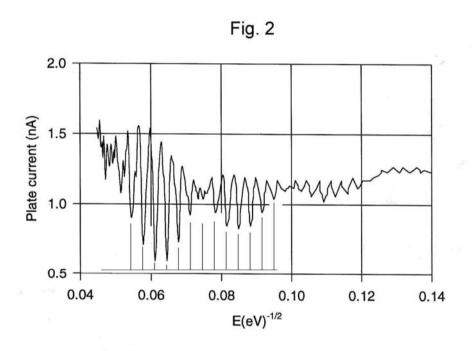


Fig.3

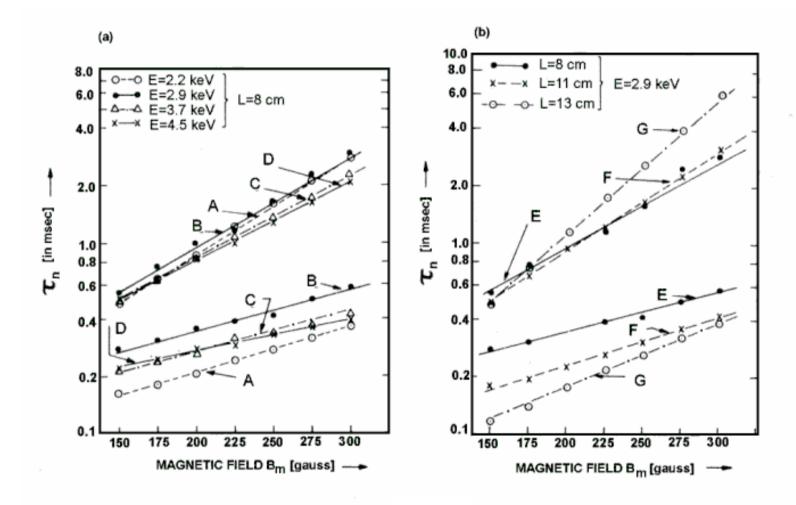


Fig. 1

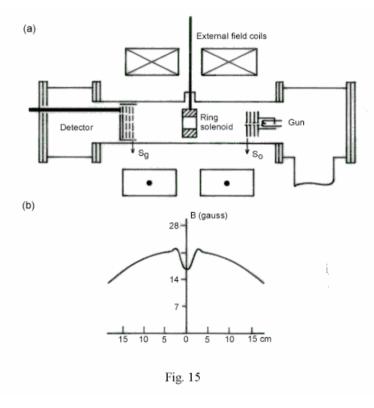


Fig.4a

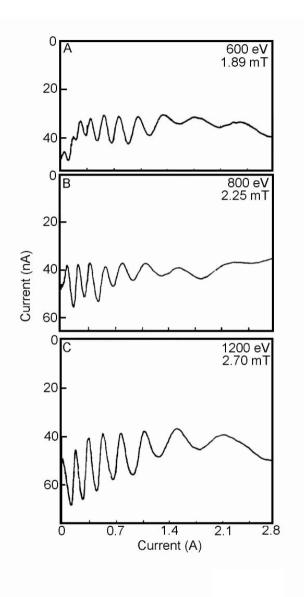


Fig 4b