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Edited by A. Dold and B. Eckmann

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A. Truman I. M. Davies (Eds.)

Stochastic Mechanics and Stochastic Processes

Proceedings, Swansea 1986

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Stochastic Mechanics and Stochastic Processes

Proceedings of a Conference
held in Swansea, U.K., Aug. 4–8, 1986

Springer-Verlag
Berlin Heidelberg New York London Paris Tokyo

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Mathematics Subject Classification (1980): 60GXX, 60HXX

ISBN 3-540-50015-4 Springer-Verlag Berlin Heidelberg New York
ISBN 0-387-50015-4 Springer-Verlag New York Berlin Heidelberg

Printed in Germany

Printing and binding: Druckhaus Beltz, Hemsbach/Bergstr.
2146/3140-543210

Preface

This volume primarily contains papers presented at the meeting entitled 'Stochastic Mechanics and Stochastic Processes' held in Swansea from 4 August to 8 August 1986. Also included in the volume are some related papers, not presented at the meeting, but in the same subject area. The topics covered herein are quite varied but all related to the central themes of the meeting, including large deviations and statistical mechanics, Nelson's stochastic mechanics and quantum diffusions, simulations of Brownian Motions and stochastic flows. The meeting was most worthwhile both in the quality of the talks given and the level of discussion generated on the subject of stochastic processes and stochastic mechanics.

Most of the papers herein are reasonably self-contained and should be readily accessible to researchers in this field. For beginning students in Nelson's stochastic mechanics we recommend that they start by reading the first paper in this volume by Batchelor and Truman, which deals with stochastic mechanics for excited states of a system with finitely many degrees of freedom. Some of the corresponding stochastic flows are discussed in the paper by Chappell and Elworthy, where new results are given for their Lyapunov exponents. There are related papers by Yasue, Durran and Williams and Steele. Zambrini's paper includes new results for Bernstein processes and stochastic mechanics. An interesting new treatment of stochastic mechanics for systems with infinitely many degrees of freedom (quantum fields) is given in the paper by Carlen. Supersymmetry is discussed in the paper by Haba.

There is an excellent expository account of large deviations in statistical mechanics by Lewis, and two papers by Lewis and co-workers in statistical mechanics itself. There have been exciting new developments in this area recently. An introduction to the algebraic theory of quantum diffusions is given in the paper by Hudson. New analytical results for stochastic processes are given in the papers by Kifer, McGill, McGregor and Watling.

It is a pleasure to thank Brian Davies, of King's College London, and Nick Bingham, of Royal Holloway, for their assistance in helping to organise the meeting and in producing this volume. We are grateful to the SERC for financial support through research grant GR/D/88847. We should like to thank Mrs E. Evans, Mrs M. Prowse and Mrs E. Williams for their patience and application in typing some of the papers. Last but far from least we would like to thank the referee for his important contribution.

A. Truman and I.M. Davies
Swansea

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ON FIRST HITTING TIMES IN STOCHASTIC MECHANICS

by

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1. A Resumé of Stochastic Mechanics

The Schrödinger equation for a particle Q of mass m subject to a force $-\nabla V$ in $\mathbb{R}^d$ is equivalent to

$$i\hbar\psi^* \frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\psi^*\Delta_x\psi + \psi^* V\psi, \tag{1}$$

where * denotes the complex conjugate and $\hbar$ is Planck's constant divided by 2π. Here $\psi = \psi(\underset{\sim}{x},t)$ is the quantum mechanical wave-function and the time $t \in \mathbb{R}^+$, the positive reals, and $\underset{\sim}{x} \in \mathbb{R}^d$, d-dimensional Euclidean configuration space.

Since V is real-valued, equating imaginary parts of the above equation gives the continuity equation

$$\frac{\partial\rho}{\partial t} + \operatorname{div} \underset{\sim}{j} = 0, \tag{2}$$

where $\rho = \psi^*\psi$ is the quantum mechanical particle density and $\underset{\sim}{j} = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*)$ is the probability current. The last equation merely expresses the conservation of particle number in that, for the state ψ, the probability that Q is in A at time t is given by

$$\mathbb{P}\{Q \in A \text{ at time } t\} = \int_A \rho(\underset{\sim}{x},t)dx, \tag{3}$$

for each Borel set $A \subset \mathbb{R}^d$.

Following Nelson [6],[7], introduce the real-valued functions R and S defined by $\psi = e^{R+iS}$, so that $\rho = e^{2R}$ and $\underset{\sim}{j} = (\frac{\hbar}{m}\nabla S)e^{2R}$. We can then deduce from the continuity equation that

$$\frac{\partial\rho}{\partial t} = \operatorname{div}(-\frac{\hbar}{m}\nabla Se^{2R}) = \operatorname{div}(\frac{\hbar}{2m}\nabla e^{2R} - \frac{\hbar}{m}\nabla(R+S)e^{2R}) \tag{4}$$

i.e.

$$\frac{\partial\rho}{\partial t} = \operatorname{div}(\nu\nabla\rho - \underset{\sim}{b}\rho), \tag{5}$$

for $\nu = \frac{\hbar}{2m}$ and $\underset{\sim}{b} = \frac{\hbar}{m}\nabla(R+S)$.

The last equation is just the forward Kolmogorov equation for the density ρ for the diffusion $\underset{\sim}{X}$ satisfying

$$d\underset{\sim}{X} = \underset{\sim}{b}(\underset{\sim}{X}(t),t)dt + \left(\frac{\hbar}{m}\right)^{\frac{1}{2}} d\underset{\sim}{B}(t), \tag{6}$$

where the forward drift $\underset{\sim}{b} = \frac{\hbar}{m}\underset{\sim}{\nabla}(R+S)$, $\underset{\sim}{B} = (B_1, B_2, \ldots, B_d)$ in cartesians, with $\mathbb{E}\{B_i(t)B_j(s)\} = \delta_{ij}\min(s,t)$, for $i,j = 1,2,\ldots,d$, $\underset{\sim}{B}$ being a $BM(\mathbb{R}^d)$ process. Moreover, equating the real parts of Eq. (1) gives for $\psi = e^{R+iS}$

$$\frac{\partial S}{\partial t} = \frac{\hbar}{2m}(|\underset{\sim}{\nabla}R|^2 - |\underset{\sim}{\nabla}S|^2 + \Delta R) - \frac{V}{\hbar}. \tag{7}$$

Nelson's remarkable discovery was that the last equation embodies a dynamical principle for the diffusion $\underset{\sim}{X}$.

To see this Nelson defines the mean forward and backward time derivatives $D_\pm$ by

$$D_\pm f(\underset{\sim}{X}(t),t) = \lim_{h\downarrow 0} \mathbb{E}\left\{\frac{f(\underset{\sim}{X}(t\pm h),t\pm h) - f(\underset{\sim}{X}(t),t)}{\pm h}\middle|\underset{\sim}{X}(t)\right\}. \tag{8}$$

Then it follows from Eq. (6) that

$$D_+\underset{\sim}{X}(t) = \underset{\sim}{b}(\underset{\sim}{X}(t),t) = \frac{\hbar}{m}\underset{\sim}{\nabla}(S+R)(\underset{\sim}{X}(t),t) \tag{9}$$

and from Itô's formula that for sufficiently regular f

$$D_+ f(\underset{\sim}{X}(t),t) = \left(\frac{\partial f}{\partial t} + \underset{\sim}{b}.\underset{\sim}{\nabla}f + \frac{\hbar}{2m}\Delta f\right)(\underset{\sim}{X}(t),t). \tag{10}$$

Nelson went on to show that for sufficiently regular functions g and h

$$\frac{d}{dt}\mathbb{E}(g(\underset{\sim}{X}(t))h(\underset{\sim}{X}(t))) = \mathbb{E}(g(\underset{\sim}{X}(t))D_-h(\underset{\sim}{X}(t))) + \mathbb{E}(D_+g(\underset{\sim}{X}(t))h(\underset{\sim}{X}(t))) \tag{11}$$

(see e.g. p. 98 Ref (6)).

We can now establish Nelson's result. Firstly, from above, for any $f \in C_0^\infty(\mathbb{R}^d)$, for $i = 1,2,\ldots,d$,

$$\frac{d}{dt}\mathbb{E}\{f(\underset{\sim}{X}(t))X_i(t)\} = \mathbb{E}\{f(\underset{\sim}{X}(t))D_-X_i(t)\} + \mathbb{E}\{X_i(t)(\frac{\hbar}{m}(\underset{\sim}{\nabla}R + \underset{\sim}{\nabla}S).\underset{\sim}{\nabla}f + \frac{\hbar}{2m}\Delta f)(\underset{\sim}{X}(t),t)\}, \tag{12}$$

where $\underset{\sim}{X} = (X_1, X_2, \ldots, X_d)$ in cartesians. Since $\mathbb{E}(g(\underset{\sim}{X}(t),t)) = \int_{\mathbb{R}^d} e^{2R(\underset{\sim}{x},t)} g(\underset{\sim}{x},t)dx$, integrating by parts, using the identity, for $i = 1,2,\ldots,d$,

$$-e^{-2R(\underset{\sim}{x},t)}\operatorname{div}\{x_i\underset{\sim}{\nabla}R(\underset{\sim}{x},t)e^{2R(\underset{\sim}{x},t)}\} + 2^{-1}e^{-2R(\underset{\sim}{x},t)}\Delta(x_i e^{2R(\underset{\sim}{x},t)}) = \nabla_i R(\underset{\sim}{x},t), \tag{13}$$

for $\underset{\sim}{\nabla}R = (\nabla_1 R, \nabla_2 R, \ldots, \nabla_d R)$ in cartesians, we obtain for each $f \in C_0^\infty(\mathbb{R}^d)$

$$\frac{d}{dt}\mathbb{E}\{f(\underset{\sim}{X}(t))X_i(t)\} = \mathbb{E}\{f(\underset{\sim}{X}(t)D_-X_i(t)\} + \frac{\hbar}{m}\mathbb{E}\{X_i(t)(\underset{\sim}{\nabla}S.\underset{\sim}{\nabla}f)(\underset{\sim}{X}(t),t)\} + \frac{\hbar}{m}\mathbb{E}\{(\nabla_i R)f(\underset{\sim}{X}(t),t)\}. \tag{14}$$

But Ehrenfest's theorem for the quantum mechanical state $\psi = e^{R+iS}$ gives for sufficiently regular g

$$\frac{d}{dt}\mathbb{E}(g(\underset{\sim}{X})) = \frac{\hbar}{m}\mathbb{E}((\underset{\sim}{\nabla}g).(\underset{\sim}{\nabla}S)(\underset{\sim}{X},t)). \tag{15}$$

Hence, setting $g(\underset{\sim}{X}) = f(\underset{\sim}{X})X_i$, we obtain

$$\frac{d}{dt}\mathbb{E}(f(\underset{\sim}{X})X_i) = \frac{\hbar}{m}\mathbb{E}(\nabla_i S(\underset{\sim}{X},t)f(\underset{\sim}{X})) + \frac{\hbar}{m}\mathbb{E}(X_i\underset{\sim}{\nabla}S(\underset{\sim}{X},t).\underset{\sim}{\nabla}f(X)), \tag{16}$$

for $i = 1,2,\ldots,d$.

Comparing this with Eq. (14) above, we see that necessarily

$$D_-X_i(t) = \frac{\hbar}{m}(\nabla_i S - \nabla_i R)(\underset{\sim}{X}(t),t) \tag{17}$$

for $i = 1,2,\ldots,d$. Hence, the backward drift $D_-\underset{\sim}{X}(t)$ is given by

$$D_-\underset{\sim}{X}(t) = \frac{\hbar}{m}(\underset{\sim}{\nabla}S - \underset{\sim}{\nabla}R)(\underset{\sim}{X}(t),t) \tag{18}$$

and from Itô's formula

$$D_-f(\underset{\sim}{X}(t),t) = (\frac{\partial f}{\partial t} + \frac{\hbar}{m}(\underset{\sim}{\nabla}S - \underset{\sim}{\nabla}R).\nabla f - \frac{\hbar}{2m}\Delta f)(\underset{\sim}{X}(t),t). \tag{19}$$

Nelson's amazing discovery now follows from Eqs. (9), (10), (18) and (19). After a tedious calculation we obtain

$$\frac{m}{2}(D_-D_+ + D_+D_-)\underset{\sim}{X}(t) = \{\hbar\underset{\sim}{\nabla}\frac{\partial S}{\partial t} - \frac{\hbar^2}{2m}\underset{\sim}{\nabla}(|\underset{\sim}{\nabla}R|^2 - |\underset{\sim}{\nabla}S|^2 + \Delta R)\}(\underset{\sim}{X}(t),t), \tag{20}$$

or from Eq. (7)

$$\frac{m}{2}(D_-D_+ + D_+D_-)\underset{\sim}{X}(t) = -\underset{\sim}{\nabla}V(\underset{\sim}{X}(t)). \tag{21}$$

This is the Nelson-Newton law i.e. a stochastic version of Newton's second law of motion

$$\text{Force} = \text{Mass} \times \text{Acceleration}. \tag{22}$$

Therefore, we have seen that the net content of the Schrödinger equation for the state $\psi = e^{R+iS}$ is just the Kolmogorov equation for the diffusion $\underset{\sim}{X}$ with drift $\frac{\hbar}{m}(\underset{\sim}{\nabla}R + \underset{\sim}{\nabla}S)$ and the dynamical principle for $\underset{\sim}{X}$ contained in Eq. (21). This suggests that the sample paths of the diffusion $\underset{\sim}{X}$ have some physical significance. We investigate this for the stationary states of the Coulomb problem below presenting some new results for first hitting times. We do not give all the details of the proofs here and we refer the reader to the original references for details. (See

Refs. (2) and (3)).

2. First Hitting Times for Ground States of Spherically Symmetric Potentials

We consider Nelson diffusions corresponding to ground state solutions of the Schrödinger equation for a quantum mechanical Hamiltonian $H = (-\frac{\hbar^2}{2m}\Delta + V)$, a self-adjoint linear operator on some appropriate domain in $L^2(\mathbb{R}^d)$. We specialize to the case $d = 3$ and further we assume that the potential V is spherically symmetric, $V = V(|\underset{\sim}{x}|)$, for $\underset{\sim}{x} \in \mathbb{R}^3$, $|\cdot|$ being the Euclidean norm.

Let $\Psi_E(\underset{\sim}{x},t) = \Psi_t^E(\underset{\sim}{x}) \in L^2(\mathbb{R}^3)$ be such a ground state with

$$\Psi_E(\underset{\sim}{x},t) = |\underset{\sim}{x}|^{-1} f_E(|\underset{\sim}{x}|)e^{-iEt/\hbar}, \tag{23}$$

E being inf spec (H). Then, as is well-known, f_E satisfies $(H_r - E)f_E = 0$, i.e. setting $x = |\underset{\sim}{x}|$,

$$\{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) - E\}f_E(x) = 0, \tag{24}$$

where $H_r = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$ is the radial Hamiltonian. We assume that V is piecewise continuous with finite discontinuities on $(0,\infty)$ so that f_E is C^2 and, of course, $f_E > 0$ on $(0,\infty)$ and $f_E(0) = 0$.

A straight-forward application of Itô's formula yields for the Nelson diffusion $\underset{\sim}{X}$ corresponding to the state Ψ_E

$$d|\underset{\sim}{X}| = \frac{\hbar}{m}\frac{d}{d|\underset{\sim}{X}|}\ln f_E(|X|)\,dt + (\frac{\hbar}{m})^{\frac{1}{2}}d\beta(t), \tag{25}$$

β being a $BM(\mathbb{R})$ process. This is a one-dimensional time-homogeneous diffusion with generator

$$L_x = \frac{\hbar}{2m}\frac{d^2}{dx^2} + \frac{\hbar}{m}\frac{d}{dx}\ln f_E(x)\frac{d}{dx}. \tag{26}$$

By virtue of Eq. (24) the radial diffusion $|\underset{\sim}{X}|$ satisfies the Nelson-Newton law

$$\frac{m}{2}(D_+D_- + D_-D_+)|\underset{\sim}{X}(t)| = -\frac{d}{d|X|}V(|X|(t)). \tag{27}$$

Moreover, since for any C^2 function f,

$$f_E^{-1}(H_r - E)(f_E f) = f_E^{-1}\{-\frac{\hbar^2}{2m}(f_E f'' + 2f_E' f' + f_E'' f) + (V-E)f_E f\} = -\hbar L f, \tag{28}$$

f_E being positive, we obtain formally at least

$$p_t(x,y) = f_E^{-1}(x)\exp\{-\frac{t}{\hbar}(H_r - E)\}(x,y)f_E(y), \tag{29}$$

p_t being the transition density for $|\underset{\sim}{X}|$, $\exp\{-\frac{t}{\hbar}(H_r - E)\}(x,y)$ being the appropriate heat kernel. For convenience now set $\hbar = m = 1$.

We now set about finding the distribution of $\tau_x(a)$:

$$\tau_x(a) = \inf\{s > 0 : |\underset{\sim}{X}(s)| = a,\ |\underset{\sim}{X}(0)| = x\}, \tag{30}$$

the first hitting time of the level a for the process starting at x. The key result here is

$$\mathbb{E}\{\exp(-\lambda\tau_x(a))\} = f_E^{-1}(x)\,\frac{(H_r + \lambda - E)^{-1}(x,a)}{(H_r + \lambda - E)^{-1}(a,a)}\,f_E(a), \qquad (\lambda > 0), \tag{31}$$

where $(H_r + \lambda - E)^{-1}(x,a)$ is the resolvent kernel. The last identity follows because $|\underset{\sim}{X}|$ is a one-dimensional time-homogeneous diffusion. For such a diffusion to have gone from x to y in time t the first hitting time of any intermediate point a must be less than t. Since the process starts afresh from a, for each fixed x,y and any intermediate a,

$$p_t(x,y) = \int_0^t g(x,a;u)\,p_{t-u}(a,y)\,du, \tag{32}$$

where $g(x,a;u)du = \mathbb{P}\{\tau_x(a) \in (u,u+du)\}$. The desired identity follows by taking Laplace transforms and letting $y \to a$. This leads to:

PROPOSITION 1

Let $E(<0)$ be inf spec (H), where $H = -2^{-1}\Delta_x + V(|\underset{\sim}{x}|)$. For each $\lambda > 0$, let the equation

$$-2^{-1}\frac{d^2y}{dx^2} + (V(x) + \lambda - E)y = 0 \tag{33}$$

have two linearly independent C^2 solutions $f_{E-\lambda}$ and $g_{E-\lambda}$ defined by $f_{E-\lambda}(0) = 0$, $f'_{E-\lambda}(0) = 1$, $g_{E-\lambda}(0) = 1$, $g'_{E-\lambda}(0) = 0$. (This will be the case e.g. if $x^2V(x)$ is analytic in a neighbourhood of the origin.) Then, if V is piecewise continuous, with $V(x) \to 0$ as $x \to \infty$, for $\tau_x(a)$ the first hitting time for the ground state radial process, for the Hamiltonian H, for $x < a$,

$$\mathbb{E}\{\exp(-\lambda\tau_x(a))\} = f_{E-\lambda}(x)f_E(a)/f_{E-\lambda}(a)f_E(x), \tag{34}$$

whilst for $x > a$

$$\mathbb{E}\{\exp(-\lambda\tau_x(a))\} = h_{E-\lambda}(x)f_E(a)/h_{E-\lambda}(a)f_E(x), \tag{35}$$

h being the unique solution of Eq. (33), which is exponentially decreasing at infinity.

The above result yields:

COROLLARY 1

Let $x > a$ and further let V have compact support with $\operatorname{supp} V \subset [0,a)$. Then for the radial ground state process with energy $E(<0)$

$$\mathbb{E}\{\exp(-\lambda\tau_x(a))\} = \exp(-\sqrt{(-2(E-\lambda))}(x-a))\exp(+\sqrt{(-2E)}(x-a)). \tag{36}$$

Thus,

$$\mathbb{P}(\tau_x(a) \in ds) = (2\pi)^{-\frac{1}{2}}|a-x|s^{-3/2}\exp\{Es - \frac{(x-a)^2}{2s} + \sqrt{(-2E)}(x-a)\}ds. \tag{37}$$

In this case, therefore, for $x > a$, with $\operatorname{supp} V \subset [0,a)$, the distribution of $\tau_x(a)$ is the same as that for Brownian motion with a constant drift $-\sqrt{(-2E)}$ (see e.g. Ref. (10)). The last example is atypical in that one has an explicit formula for the distribution of $\tau_x(a)$. More typical is the next example.

Example 1 (Spherical Square Well Ground State)

Let $V(\underset{\sim}{x}) = -V_o$, for $|\underset{\sim}{x}| < r_o$, $V(\underset{\sim}{x}) = 0$, otherwise. The ground state energy E and ground state wave-function f_E are defined by

$$f_E(|\underset{\sim}{x}|) = \begin{cases} \sinh(\sqrt{(-2(E+V_o))}|\underset{\sim}{x}|), & |\underset{\sim}{x}| < r_o, \\ B\exp(-\sqrt{(-2E)})|\underset{\sim}{x}|), & |\underset{\sim}{x}| > r_o, \end{cases}$$

where E and B satisfy

$$\sinh(\sqrt{(-2(E+V_o))}r_o) = B\exp(-\sqrt{(-2E)}r_o),$$

$$\frac{d}{dr_o}\sinh(\sqrt{(-2(E+V_o))}r_o) = \frac{d}{dr_o}B\exp(-\sqrt{(-2E)}r_o).$$

Let $x < a < r_o$. Then

$$\mathbb{E}\{\exp(-\lambda\tau_x(a))\} = \frac{\sinh(\sqrt{(-2(E+V_o-\lambda))}x)\sinh(\sqrt{(-2(E+V_o))}a)}{\sinh(\sqrt{(-2(E+V_o-\lambda))}a)\sinh(\sqrt{(-2(E+V_o))}x)}. \tag{38}$$

Similar results can be obtained for other values of x and a. A more interesting physical example is:

Example 2 (Coulomb Problem Ground State)

Let $V(\underset{\sim}{x}) = -Ze^2/|\underset{\sim}{x}|$. The ground state energy $E = -1/2a_o^2$, a_o being the Bohr radius $1/Ze^2$. The corresponding ground state wave-function is $f_E(|\underset{\sim}{x}|) = |\underset{\sim}{x}|\exp(-|\underset{\sim}{x}|/a_o)$. In this case we obtain

$$\mathbb{E}\{\exp(-\lambda\tau_r(a))\} = \left(\frac{a}{r}\right) \exp\left(\frac{r-a}{a_o}\right) \frac{W_{\frac{1}{\kappa},\frac{1}{2}}\left(\frac{2\kappa r}{a_o}\right)}{W_{\frac{1}{\kappa},\frac{1}{2}}\left(\frac{2\kappa a}{a_o}\right)} \quad (r \geq a), \tag{39}$$

and

$$\mathbb{E}\{\exp(-\lambda\tau_r(a))\} = \left(\frac{a}{r}\right) \exp\left(\frac{r-a}{a_o}\right) \frac{M_{\frac{1}{\kappa},\frac{1}{2}}\left(\frac{2\kappa r}{a_o}\right)}{M_{\frac{1}{\kappa},\frac{1}{2}}\left(\frac{2\kappa a}{a_o}\right)} \quad (r \leq a), \tag{40}$$

a_o being the Bohr radius and $\kappa = \sqrt{(1 + 2a_o^2\lambda)}$, W and M being Whittaker functions. (See Ref. (3)).

Needless to say we cannot find the inverse Laplace transforms for either of above examples. We choose a different approach below.

3. Expected Values of First Hitting Times

We begin with a minor extension of an analytical result of Mandl (see Ref. (5)). We use the same notation as above.

PROPOSITION 2

Let $f_E(>0)$ be such that $b(x) = f_E'(x)/f_E(x)$ is Lipschitz continuous on $(0,\infty)$, 0 and ∞ being entrance and natural boundaries for the radial gound-state diffusion $|\underset{\sim}{X}|$ with generator $L_x = 2^{-1}\frac{d^2}{dx^2} + b(x)\frac{d}{dx}$. Then for the radial ground state process $v(x) = \mathbb{E}(\tau_x(a))$ satisfies

$$L_x v(x) = 2^{-1}v''(x) + b(x)v'(x) = -1, \tag{41}$$

together with the boundary conditions $v(a) = 0$ and $\lim_{x\downarrow 0} f_E^2(x)v'(x) = 0$ for $x < a$ and $\lim_{x\uparrow\infty} f_E^2(x)v'(x) = 0$ for $x > a$.

The proof of this relies heavily on the methods of Mandl (see Refs. (5) and (3)). Here we content ourselves with a formal explanation of what is going on. First we differentiate with respect to λ the equation

$$(H_r + \lambda - E) f_{E-\lambda} = 0,$$

yielding

$$\frac{df}{d\lambda} E - \lambda = -(H_r + \lambda - E)^{-1} f_{E-\lambda}. \tag{42}$$

If we assume $v(x) = \mathbb{E}(\tau_x(a)) = \lim_{\lambda \downarrow 0} \frac{d}{d\lambda} \mathbb{E}\{\exp(-\lambda\tau_x(a))\}$ the last identity leads to the desired conditions on v.

To see this refer back to the results of the last section for $x < a$, using $f_{E-\lambda} \to f_E$ as $\lambda \to 0$,

$$-\lim_{\lambda \downarrow 0} \frac{d}{d\lambda} \mathbb{E}\{\exp(-\lambda\tau_x(a))\} = \frac{(H_r - E)^{-1} f_E(x)}{f_E(x)} - \frac{(H_r - E)^{-1} f_E(a)}{f_E(a)}, \tag{43}$$

where $(H_r - E)^{-1}$ is an integral operator whose boundary conditions are to be found. Recalling that $L = -f_E^{-1}(H_r - E) f_E$, we obtain

$$L_x v(x) = -1, \quad v(a) = 0, \tag{44}$$

for $v(x) = \mathbb{E}(\tau_x(a))$. The remaining boundary condition comes about because

$$v(x) = \mathbb{E}(\tau_x(a)) = -\frac{\frac{df}{d\lambda} E - \lambda \Big|_{\lambda=0}(x)}{f_E(x)} + \frac{\frac{df}{d\lambda} E - \lambda \Big|_{\lambda=0}(a)}{f_E(a)}. \tag{45}$$

Differentiating, using the facts that $f_E(x) \to 0$ and $f_E'(x) \to 1$ as $x \to 0$, gives formally at least, for $x < a$

$$\lim_{x \downarrow 0} f_E^2(x) v'(x) = \lim_{x \downarrow 0} \frac{df}{d\lambda} E - \lambda \Big|_{\lambda=0}(x) = 0, \tag{46}$$

for a sufficiently smooth $f_{E-\lambda}(x)$ in (λ, x) in a neighbourhood of $(0,0)$, since $f_{E-\lambda}(0+) = 0$. (For further details see Ref. (3) and Batchelor's Ph.D. thesis.)

The last proposition gives for the Coulomb problem:

<u>PROPOSITION 3</u>

For the radial ground state diffusion for the Coulomb potential $V = -Ze^2/|\underset{\sim}{x}|$

$$\mathbb{E}(\tau_r(a)) = a_o^2 \int_{a/a_o}^{r/a_o} \left(1 + \frac{1}{x} + \frac{1}{2x^2}\right) dx \quad (r \geq a), \tag{47}$$

and

$$\mathbb{E}(\tau_r(a)) = a_o^2 \int_{r/a_o}^{a/a_o} \left\{\frac{1}{2x^2}(e^{2x} - 1 - 2x) - 1\right\} dx \quad (r \leq a), \tag{48}$$

$a_o = 1/Ze^2$ being the Bohr radius. Further

$\mathbb{E}(\tau_r(a) | r \in (a,\infty)$ is distributed according to quantum mechanical ground state distribution)

$$= a_o^2 \int_{a/a_o}^{\infty} (x + 1 + \frac{1}{2x})^2 e^{-2x} dx \qquad (49)$$

and

$\mathbb{E}(\tau_r(a) | r \in (0,a)$ is distributed according to quantum mechanical ground state distribution)

$$= a_o^2 \int_0^{a/a_o} \{\frac{\sinh x}{x} - (1+x)e^{-x}\}^2 dx. \qquad (50)$$

The question arises as to whether one can check any of the above results experimentally. Here we reiterate an idea in Ref. (9).

A Possible Experimental Test

If you replace the negatively charged electron in the hydrogen atom by a negatively charged pion π^-, the π^- feels only the Coulomb attraction due to the positively charged proton p^+ when at a distance exceeding $\hbar/m_\pi c$ (the pion Compton wavelength) from the nuclear proton. The reason is that the strong force governing the decay $p^+ + \pi^- \rightarrow n + \gamma$'s is of extremely short range $\sim \hbar/m_\pi c$. Therefore the $p^+\pi^-$ system cannot decay until the π^- first hits a sphere of radius $\hbar/m_\pi c$ centred at the nuclear proton.

Assume therefore that the π^- is captured into the ground state. Then, if stochastic mechanics gives the correct first hitting time, we obtain

$$\text{Expected Decay Time for Ground State of } p^+\pi^- > \frac{2\hbar^3}{m_\pi e^4} \int_{e^2/c\hbar}^{\infty} (x + 1 + \frac{1}{2x})^2 e^{-2x} dx \sim 10^{-18} \text{ secs.} \qquad (51)$$

Experiment gives:

$$\text{Expected Decay Time for } p^+\pi^- < 10^{-12} \text{ secs,}$$

which is consistent. This begs the question as to whether or not one can determine the expected first hitting times for excited states.

Denote by $a_{1,1}$ the first zero of the radial wave function for the first excited state for the Coulomb problem, i.e. the first zero of L_1^1, the Laguerre polynomial.

We let $\bar{\mathbb{E}}^1_+(\tau(a))$ denote $\mathbb{E}(\tau_r(a) | r \in (a, a_{1,1})$ is distributed according to the probability distribution of the first excited state) and $\bar{\mathbb{E}}^1_-(\tau(a))$ the corresponding expression for a diffusion initially distributed according to probability distribution of first excited state on $(0,a)$. Then the methods above yield:

PROPOSITION 4

For the first excited state for the Coulomb potential $-Ze^2/|\underset{\sim}{x}|$

$$\bar{\mathbb{E}}^1_+(\tau(a)) = \frac{8a_o^2}{(1-7e^{-2})}\int_{a/2a_o}^{1} \frac{1}{(1-\rho)^2}\{(\rho^3+\rho+1+\frac{1}{2\rho})e^{-\rho} - \frac{7e^{-(2-\rho)}}{2\rho}\}^2 d\rho \tag{52}$$

and

$$\bar{\mathbb{E}}^1_-(\tau(a)) = \frac{8a_o^2}{(1-7e^{-2})}\int_0^{a/2a_o} \frac{1}{(1-\rho)^2}\{\frac{\sinh\rho}{\rho} - (\rho^3+\rho+1)e^{-\rho}\}^2 d\rho . \tag{53}$$

Further details of the above calculation are given in Batchelor's Ph.D. thesis.

It is clearly going to be very difficult to compute analogues of the above for the n^{th} excited state. We therefore resort to asymptotic methods. (See Refs. (5) and (8)).

4. Asymptotic Results

The n^{th} excited state, with zero angular momentum, for the Coulomb problem has radial wave-function

$$f_E(x) = x\exp\left(\frac{-x}{(n+1)a_o}\right)L^1_n\left(\frac{2x}{(n+1)a_o}\right) \qquad n = 0,1,2,\ldots \tag{54}$$

$a_o = 1/Ze^2$ being the Bohr radius, L^1_n a Laguerre polynomial, the energy level $E = E_n = -\frac{Z^2e^4}{2(n+1)^2}$. The zeros of the Laguerre polynomial, labelled by $a_{i,n}$ in increasing order, are unattainable points so internodal regions $(a_{i,n}, a_{i+1,n})$ are non-communicating (see e.g. Ref. (1)). We work with wave-function f_E on $(0, a_{1,n})$ to find first hitting time of $a \sim 0$ for each energy level E_n for zero angular momentum.

We follow the methods of Mandl and Newell (see Refs. (5) and (8)) and seek a $\gamma(a) \uparrow \infty$ as $a \downarrow 0$, with

$$\lim_{a\downarrow 0} \mathbb{E}\{\exp(-\frac{\lambda\tau_x(a)}{\gamma(a)})\} = (1+\lambda)^{-1}, \tag{55}$$

for each fixed $\lambda > 0$. That such a γ exists can be seen from the results of the last section.

From Eq. (35), since $\lim_{\lambda\downarrow 0} h_{E-\lambda}(x) = f_E(x)$, for $x > a$, we obtain

$$\lim_{a\downarrow 0} \mathbb{E}\{\exp(-\frac{\lambda\tau_x(a)}{\gamma(a)})\} = \lim_{a\downarrow 0} \frac{f_E(a)}{h_{E-\frac{\lambda}{\gamma(a)}}(a)} \tag{56}$$

and from de l'Hopital's rule

$$\lim_{a\downarrow 0} \mathbb{E}\{\exp(-\frac{\lambda\tau_x(a)}{\gamma(a)})\} = \lim_{a\downarrow 0} \frac{f_E'(a)}{\left[h'_{E-\frac{\lambda}{\gamma(a)}}(a) - \lambda\frac{dh_{E-\mu}}{d\mu}\Big|_{\mu=0}(a)\,\frac{\gamma'(a)}{\gamma^2(a)}\right]}. \tag{57}$$

Hence, we obtain

$$\lim_{a\downarrow 0} \mathbb{E}\{\exp(-\frac{\lambda\tau_x(a)}{\gamma(a)})\} = (1+\lambda)^{-1}, \tag{58}$$

if γ is defined to satisfy

$$\frac{\frac{dh_{E-\mu}}{d\mu}\Big|_{\mu=0}(a)\,\frac{\gamma'(a)}{\gamma^2(a)}}{f_E'(a)} = -1. \tag{59}$$

The following is a minor extension of a result of Mandl and Newell (see Refs. (5) and (8)).

PROPOSITION 5

For the radial Nelson diffusion corresponding to the n^{th} eigenvalue E_n and eigenfunction f_{E_n}, restricted to $(0,a_{1,n})$, $\gamma(a) = 2\int_0^{a_{1,n}} f_{E_n}^2(x)\,dx \int^a f_{E_n}^{-2}(y)\,dy$ and for each fixed x

$$\lim_{a\downarrow 0} \mathbb{E}\{\exp(-\frac{\lambda\tau_x(a)}{\gamma(a)})\} = (1+\lambda)^{-1}.$$

Let us see why above γ is consistent with our Eq. (59). Firstly, if

$\lim_{a\downarrow 0} \mathbb{E}\{\exp(-\frac{\lambda\tau_x(a)}{\gamma(a)})\} = (1+\lambda)^{-1}$, for small λ, it is necessary that, as $a \sim 0$,

$$\gamma(a) \sim \mathbb{E}\{\tau_x(a)\} = \frac{-\frac{dh}{d\lambda}E-\lambda\Big|_{\lambda=0}(x)}{f_E(x)} + \frac{\frac{dh}{d\lambda}E-\lambda\Big|_{\lambda=0}(a)}{f_E(a)} . \tag{60}$$

Therefore, our equation reduces to

$$\frac{\gamma'(a)}{\gamma^2(a)} \sim -\frac{f_E'(a)}{\frac{dh}{d\lambda}E-\lambda\Big|_{\lambda=0}(a)} \sim -\frac{f_E'(a)}{f_E(a)(\gamma(a)+c(x))}, \quad \text{as } a \sim 0, \tag{61}$$

for a function $c(x)$. Evidently this equation is incapable of determining the multiplicative constant $2\int_0^{a_{1,n}} f_E^2(x)\,dx$. However, observe that $\gamma(a) = \int^a f_E^{-2}(x)\,dx$ gives

$$\frac{\gamma'(a)}{\gamma^2(a)} = \frac{f_E^{-2}(a)}{\left(\int^a f_E^{-2}(x)dx\right)^2} \sim -\frac{2f^{-3}(a)f_E'(a)}{2\int^a f_E^{-2}(x)\,dx\, f_E^{-2}(a)} = -\frac{f_E'(a)}{f_E(a)\gamma(a)}, \tag{62}$$

as it should, since $f_E(a) \sim 0$. The multiplicative constant is determined by Eq. (60). Formally then for the radial diffusion corresponding to the n^{th} eigenfunction f_{E_n}

$$\mathbb{P}(\tau_x(a) < t) \sim 1 - e^{-t/\gamma_n(a)}, \tag{63}$$

where $\gamma_n(a) = 2\int_0^{a_{1,n}} f_{E_n}^2(x)\,dx \int^a f_{E_n}^{-2}(y)\,dy$. The following proposition was discovered by Andrew Batchelor on the computer.

PROPOSITION 6

$$\lim_{n\uparrow\infty} \lim_{a\downarrow 0} \frac{\gamma^n(a)}{\gamma^0(a)} = \frac{1}{16}\int_0^{j_{1,1}} x^3 (J_1(x))^2 dx, \tag{64}$$

$j_{1,1}$ being first zero of first Bessel function J_1.

Further details are given in Refs. (2) and (3). Batchelor's computer tabulation is given at the end of this paper. There is a corresponding proposition for non-zero angular momentum states: