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STOCHASTIC MECHANICS OF MOLECULE-ION MOLECULE REACTIONS.(U)
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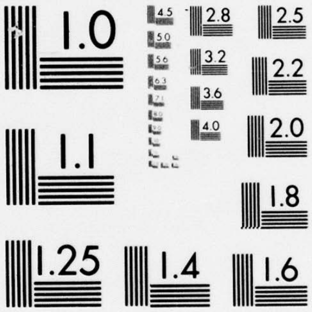

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STOCHASTIC MECHANICS OF MOLECULE-ION MOLECULE REACTIONS

⑩ Marc Mangel

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STOCHASTIC MECHANICS OF MOLECULE-ION MOLECULE REACTIONS

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June 1978

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ABSTRACT

We give a treatment of molecule-ion molecule reactions based on stochastic mechanics. Stochastic mechanics is a semiclassical theory in which one assumes that particles move as a stochastic diffusion process. It is shown that the reaction probability and reaction rate can be determined from the solution of certain partial differential equations (pde). Asymptotic solutions (for h→0) of these pde are constructed in terms of incomplete special functions. The results derived using stochastic mechanics are compared with results derived using other semiclassical approximations.

SECTION 1. INTRODUCTION

In this paper we consider the reaction of molecule ions and molecules from the viewpoint of stochastic mechanics (1). The reactions of interest are of the form

$$X^+ + YB \rightarrow XB^+ + Y, \tag{1.1}$$

e.g.

$$Ar^+ + H_2 \rightarrow ArH^+ + H. \tag{1.2}$$

These reactions may lead to the phenomenon or orbiting (see below) and have been studied by Hirschfelder et. al. (2), Gioumousis and Stevenson (3) and Ford and Wheeler (4). These workers analyzed the reaction (1.1) by using classical or semiclassical kinetic theory (2,3) or by taking the semiclassical limit of the quantum mechanical scattering theory (4). The object of major importance in these theories is the reaction cross-section, σ. Once the cross-section is known, reaction rates and probabilities can be calculated. In (4), rainbow and glory scattering are given relatively simple and general semiclassical treatments. The authors conclude that "there is no semiclassical approximation to the orbiting effect of simplicity or generality comparable to the analysis for rainbow scattering and glory scattering" (4, page 274).

In this paper, we give a general, and intuitive, semiclassical approximation to orbiting. Our approach is very different from the approach in (2-4), in that stochastic mechanics (SM) is used. One advantage of the SM approach is that reaction rates and probabilities can be calculated directly, once the stochastic problem is formulated.

In section 2, the classical mechanics problem is discussed. A discussion of the phenomenon of "orbiting" is given. In section 3, the stochastic mechanics problem is formulated. Stochastic mechanics assumes that a particle's motion is a diffusion process. The drift term of the diffusion is given by classical mechanics and the intensity of the diffusion is $\hbar/2m$, where m is the mass of the particle. The reaction probability and reaction rate are then determined by solving certain elliptic partial differential equations. The solution of these equations is discussed in section 4.

SECTION 2

CLASSICAL MECHANICS OF MOLECULE ION-MOLECULE REACTIONS

We assume that the YB molecule is chosen as the origin. The X^+ molecules approach the YB molecules with initial velocity g and asymptotic center-to-center distance b (see Fig. 1). The center-to-center distance b is called the impact parameter. We describe the collision process by the use of $r(t), \theta(t)$ coordinates, shown in Fig. 1. According to classical scattering theory (2,3,5) $r(t)$ and $\theta(t)$ evolve according to

$$\frac{d}{dt}(r)^2 = g\left[1 - \frac{b^2}{r^2} + \frac{Z\alpha e^2}{2r^4 E}\right] \qquad (2.1)$$

$$\dot{\theta} = \frac{-gb}{r^2}, \qquad (2.2)$$

where Z is the valence of X^+, α is the polarizability of YB and E is the initial energy of X^+. The molecule ion will "orbit" when $\dot{r} = 0$. The condition for $\dot{r} = 0$ is

$$1 - \frac{b^2}{r^2} + \frac{Z\alpha e^2}{2r^4 E} = 0. \qquad (2.3)$$

This equation will have a real solution only if

$$b \geq b_c \equiv \left(\frac{2Z\alpha e^2}{E}\right)^{1/4}. \qquad (2.4)$$

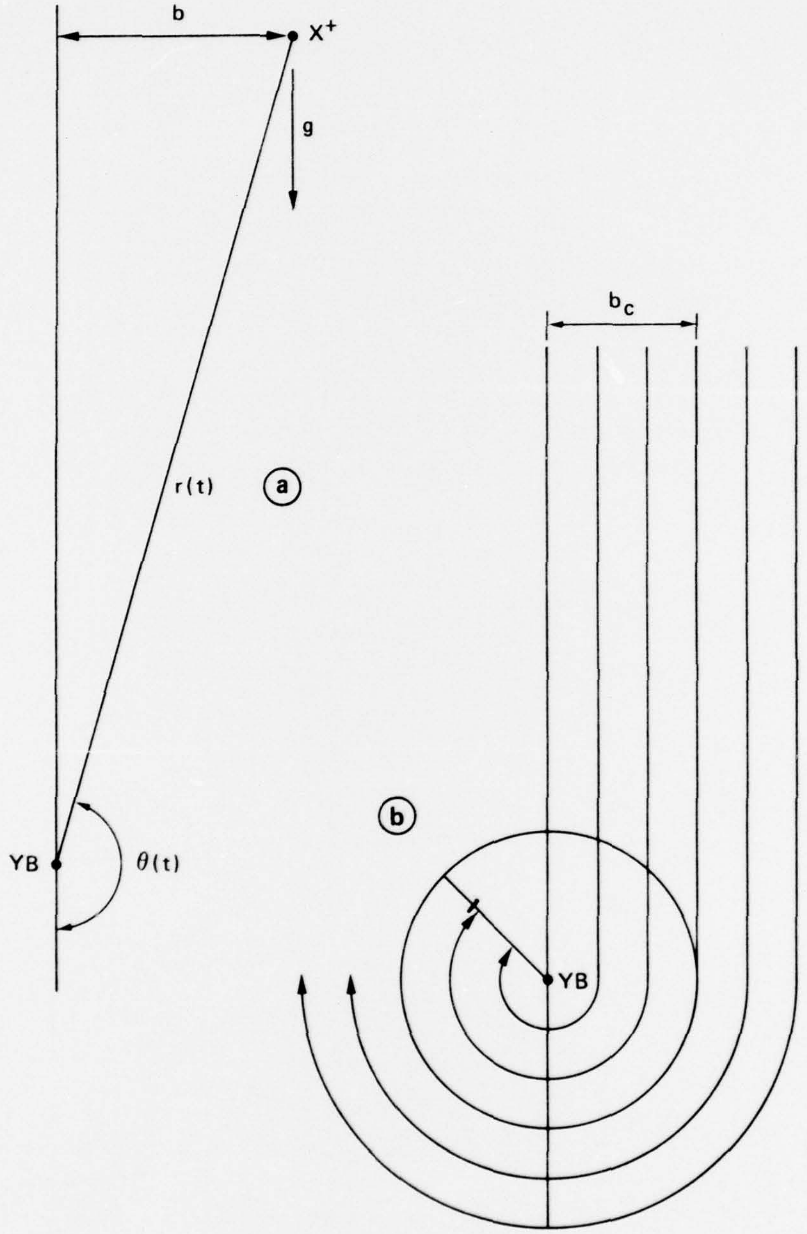

FIG. 1: GEOMETRY OF THE MOLECULE-ION MOLECULE COLLISION

We call b_c the critical value of the impact parameter. If $b < b_c$, then all solutions of (2.1, 2.2) will spiral into the origin. Once the molecule ion is within a critical reaction distance, r_x, of YB, we assume that a reaction occurs with probability 1. If $b \geq b_c$, then more interesting behavior may occur. For $b > b_c$, the molecule ion will approach YB and then fly away on a hyperbolic orbit. When $b = b_c$, however, the molecule ion will be trapped in an orbit around YB. The radius of this orbit is calculated from (2.3) and is

$$r_c = \frac{b_c}{\sqrt{2}} \qquad (2.5)$$

We view (2.1, 2.2) as a classical dynamical system. The orbit at $r = r_c$ is an unstable limit cycle (see e.g. (6) for a discussion of these terms).

In any experiment, the molecule ion X^+ will be produced according to some initial distribution of impact parameters, $\rho_0(b)$. Using the classical analysis, we see that the reaction probability will be

$$u = \int_0^{b_c} \rho_o(b)\,db. \qquad (2.6)$$

The time that it takes to enter the reaction sphere r_x from a distance r_0 is

$$T(b) = -\int_{r_o}^{r_x} \frac{g\,dr}{\left[1 - \frac{b^2}{r^2} + \frac{Z\alpha e^2}{2Er^4}\right]^{1/2}} . \tag{2.7}$$

Hence, the mean time to enter the reaction sphere, averaged over those molecules that enter is

$$\langle T(b)\rangle = \int_0^{b_c} T(b)\rho_0(b)db \tag{2.8}$$

The classical reaction rate is defined to be

$$k = \frac{1}{\langle T(b)\rangle} . \tag{2.9}$$

If the system involved more complex potentials, more complicated dynamical systems would be derived. For example, for the Lennard-Jones potential

$$V(r) = 4\eta \left[- \frac{a}{r^6} + \frac{c}{r^{12}}\right] \tag{2.10}$$

equation (2.3) is replaced by

$$1 - \frac{b^2}{r^2} + \frac{4\eta}{E}\left\{- \frac{a}{r^6} + \frac{c}{r^{12}}\right\} = 0. \tag{2.11}$$

In this case, stable and unstable limit cycles will appear in the classical dynamics (Fig. 2).

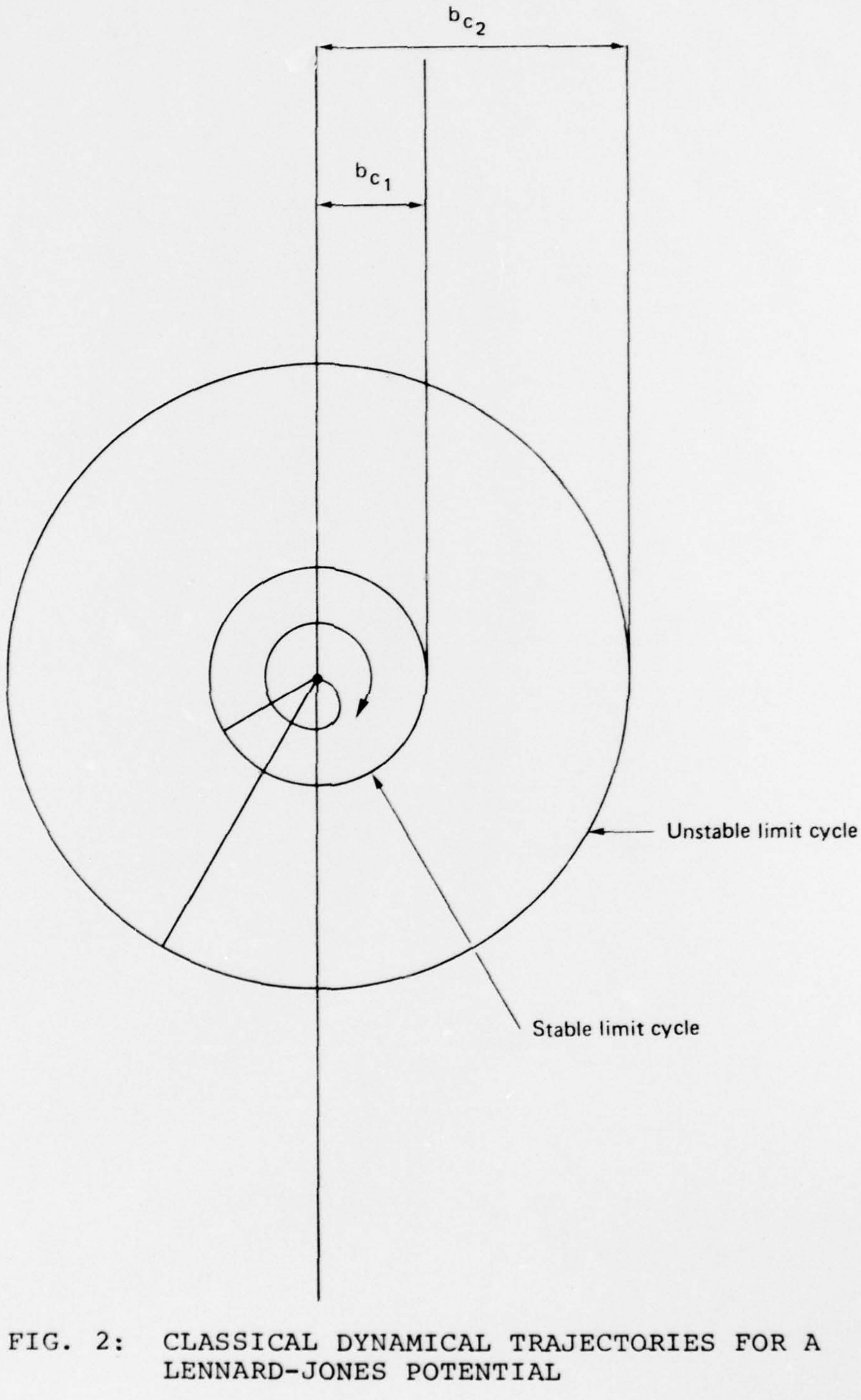

FIG. 2: CLASSICAL DYNAMICAL TRAJECTORIES FOR A LENNARD-JONES POTENTIAL

SECTION 3. STOCHASTIC MECHANICS

In order to convert the classical theory of section 2 to a semiclassical theory, we assume that $\tilde{r}(t)$ and $\tilde{\theta}(t)$ are stochastic diffusion processes (1). Specifically assume that $\tilde{r}(t)$ and $\tilde{\theta}(t)$ satisfy the Ito equations

$$d\tilde{r} = \frac{g}{2r}\left(1 - \frac{b^2}{\tilde{r}^2} + \frac{Z\alpha e^2}{2E\tilde{r}^4}\right) dt + \sqrt{\frac{\hbar}{m}}\, dW_1 \tag{3.1}$$

$$d\tilde{\theta} = -\frac{bg}{\tilde{r}^2}dt + \sqrt{\frac{\hbar}{m}}\, dW_2 \; . \tag{3.2}$$

In (3.1, 2) W_1 and W_2 are independent Brownian motion processes. Namely $E(dW) = 0$, $E(dW^2) = dt$ and the increments dW are normally distributed.

The picture provided by stochastic mechanics is this: particles move according to classical mechanics and are continually perturbed by quantum noise.

Let $u(r,\theta)$, $T(r,\theta)$ be defined by

$$u(r,\theta) = \Pr\Big\{ X^+ \text{ enters } r_x \text{ rather than approaching } r = \infty$$

$$= \big| \tilde{r}(0) = r, \tilde{\theta}(o) = \theta \Big\} \tag{3.3}$$

$$T(r,\theta) = E\Big\{ t\text{: } \tilde{r}(t) \leq r_x,\ r(s) > r_x \text{ for } s < t \,\big|\, \tilde{r}(0) = r$$

$$\tilde{\theta}(0) = \theta \Big\} \tag{3.4}$$

The function $u(r,\theta)$ is the reaction probability as a function of initial position (and thus impact parameter). $T(r,\theta)$ is the average time that it takes a X^+ particle to enter the reaction sphere of YB, given the initial position. Hence, after an appropriate averaging over initial position, $T(r,\theta)$ is a measure of the rate of the reaction.

In a standard way (1,7) it can be shown that u and T satisfy the following deterministic partial differential equations:

$$\frac{\hbar}{2m}(u_{rr} + u_{\theta\theta}) - \frac{bg}{r^2}u_\theta + \frac{g}{2r}\left(1 - \frac{b^2}{r^2} + \frac{Z\alpha e^2}{2Er^4}\right)u_r = 0 \qquad (3.5)$$

$$\frac{\hbar}{2m}(T_{rr} + T_{\theta\theta}) - \frac{bg}{r^2}T_\theta + \frac{g}{2r}\left(1 - \frac{b^2}{r^2} + \frac{Z\alpha e^2}{2Er^4}\right)T_r = -1. \qquad (3.6)$$

In (3.5,6) subscripts indicate partial derivatives.

The boundary conditions for (3.5) are

$$u(r_x,\theta) = 1 \qquad u(\infty,\theta) = 0 \qquad u(r,\theta + 2\pi) = u(r,\theta). \qquad (3.7)$$

The boundary conditions for (3.6) are

$$T(r_x,\theta) = 0 \qquad \lim_{r\to\infty} T_r(r,\theta) = 0$$

$$T(r,\theta + 2\pi) = T(r,\theta). \qquad (3.8)$$

Once $u(r,\theta)$, $T(r,\theta)$ are known, the overall reaction probability and rate are obtained by averaging over the initial distribution

$$\nu = \int u(r,\theta)\rho_0(r,\theta)drd\theta \tag{3.9}$$

$$k = \left[\int T(r,\theta)\rho_0(r,\theta)drd\theta\right]^{-1} . \tag{3.10}$$

Equations (3.5, 6) are singular perturbation problems, since $\hbar/2m$ is small.

SECTION 4. ASYMPTOTIC SOLUTIONS

It is clear that quantum effects will be most noticable for $r \approx r_c$ (r_c given by 2.5). Thus, the region of major interest when constructing solutions of (3.5, 3.6) is a vicinity of the unstable limit cycle $r = r_c$. Elsewhere (8), we have shown how to construct solutions of (3.5, 3.6). We consider (3.5) first.

An asymptotic solution of (3.5) is (8)

$$u(r,\theta) = g(r,\theta,\frac{\hbar}{2m})E(\psi(r,\theta)/\sqrt{\hbar/2m}\,) \qquad (4.1)$$

$$+\left(\frac{\hbar}{2m}\right)^{1/2} f(r,\theta,\hbar/2m)E'(\psi(r,\theta)/\sqrt{\hbar/2m}\,).$$

In (4.1), $\psi(r,\theta)$, g and f are to be determined. We assume that

$$g(r,\theta,\hbar/2m) = \sum_k (\hbar/2m)^k g^k(r,\theta) \qquad (4.2)$$

$$f(r,\theta,\hbar/2m) = \sum_k (\hbar/2m)^k f^k(r,\theta). \qquad (4.3)$$

Finally, $E(z)$ appearing in (4.1) is the error integral:

$$E(z) = \int^z e^{-s^2/2} ds \qquad z_0 \leq z \leq z_1. \qquad (4.4)$$

The error intergral satisfies

$$\frac{d^2E}{dz^2} = -z\,\frac{dE}{dz}\,. \tag{4.5}$$

In order to evaluate ψ,g and f, derivatives of (4.1) are evaluated and substituted into (3.5). When evaluating derivatives, (4.5) is used to replace $E''(\psi/\sqrt{\hbar/2m})$ by $-\left(\psi\sqrt{(\hbar/2m)}\right)E'\left(\psi/\sqrt{\hbar/2m}\right)$ After substitution into (3.5), terms are collected according to powers of $(\hbar/2m)$. The coefficients of the various powers of $(\hbar/2m)$ are set equal to zero, yielding equations for ψ, g^k and f^k. Here we only discuss ψ, g^0 and f^0, which gives the leading term in (4.1). Other terms are treated in an analogous fashion (8).

We set

$$b^\theta = \frac{-bg}{r^2} \tag{4.6}$$

$$b^r = \frac{g}{2r}\left(1 - \frac{b^2}{r^2} + \frac{Z\alpha e^2}{2Er^4}\right), \tag{4.7}$$

so that the classical equations are $\dot{\theta} = b^\theta$, $\dot{r} = b^r$. The leading term in the asymptotic solution of (3.5) is $0\left((\hbar/2m)^{-1/2}\right)$. It vanishes if $\psi(r,\theta)$ satifies

$$b^r\psi_r + b^\theta\psi_\theta - \psi(\psi_r^2 + \psi_\theta^2) = 0. \tag{4.8}$$

The $0(1)$ term vanishes if $g^0(r,\theta)$ satisfies

$$b^r g^0_r + b^\theta g^0_\theta = 0. \tag{4.9}$$

The $0\left((h/2m)^{1/2}\right)$ term vanishes if $f^0(r,\theta)$ satifies:

$$\begin{aligned} b^r f^0_r + b^\theta f^0_\theta + g^0(\psi_{rr} + \psi_{\theta\theta}) + 2\left[g^0_r\psi_r + g^0_\theta\psi_\theta\right] \\ - 2(f^0_r\psi_r + f^0_\theta\psi_\theta)\psi - f^\theta\left((\psi\psi_r)_r + (\psi\psi_\theta)_\theta\right) = 0 \end{aligned} \tag{4.10}$$

We first consider (4.8). The region of major interest is a vicinity of the unstable limit cycle, so that we will obtain $\psi(r,\theta)$ in a vicinity of the limit cycle. Since r_c corresponds to an orbit, $b^r(r_c) = 0$. Intuition suggests that we set $\psi_\theta(r_c,\theta) = 0$. Then (4.8) indicates that $\psi = 0$ on r_c. We can determine $\psi(r,\theta)$ in a vicinity of r_c by Taylor expansion, once $\psi_r(r_c,\theta)$ is known. If (4.8) is differentiated with respect to r and evaluated on $r = r_c$, we obtain

$$b^\theta\psi_{\theta r} + b^r_{,r}\psi_r - \psi^3_r = 0. \tag{4.11}$$

Now $b^\theta\,\partial/\partial\theta + b^r\,\partial/\partial r = d/dt$, where t measures "time" along the limit cycle. Since $b^r(r_c) = 0$ and $\theta(t) = -(bg/r_c^2)t + \theta_0$ on $r = r_c$, we obtain

$$\frac{d}{dt}\psi_r + b^r_{,r}\psi_r - \psi^3_r = 0. \tag{4.12}$$

In terms of θ, we obtain

$$\frac{-bg}{r_c^2} \frac{d}{d\theta} \psi_r + b^r_{,r} \psi_r - \psi_r^3 = 0. \tag{4.13}$$

The periodic solution of (4.13) gives $\psi_r(r_c,\theta)$. Once this derivative is known, $\psi(r,\theta)$ can be determined in a vicinity of the limit cycle. A more accurate procedure for the determination of $\psi(r,\theta)$ would involve the solution of (4.8) by the method of characteristics (see (8)). Since b^r is independent of θ, the periodic solution of (4.13) is simply

$$\psi_r = (b^r_{,r})^{1/2}. \tag{4.14}$$

Equation (4.9) indicates that g^0 is constant on classical trajectories. We set g^0 identically constant, and determine its value b by requiring $g^0 E(\psi(r,\theta)/\sqrt{(\hbar/2m)}$ asymptotically satisfy the boundary conditions. From equation (4.10), we can derive an equation for f^0 on the limit cycles requiring that $f^0(\theta + 2\pi) = f^0(\theta)$. Once f^0 is known, the first term of the asymptotic solution of (3.5) is known. From (4.1)

$$u(r,\theta) \sim g^0 \, E\left((b^r_{,r})^{1/2}(r - r_c)/\sqrt{\hbar/2m}\right). \tag{4.15}$$

Hence, the parameter $\tau = (b^{r}_{,r})^{1/2}$ measures the rate of fall off of reaction probability as a function of the physical parameters:

$$\tau = g\left[\frac{b^2}{r_c^2} - \frac{Z\alpha e^2}{Er_c^6}\right] \tag{4.16}$$

The result (4.16) is a SM analogue to equation (4.3) of Ford and Wheeler (4).

The solution of equation (3.3), for $T(r,\theta)$ can be given in a form analogous to (4.1):

$$\begin{aligned} T(r,\theta) &= g(r,\theta,\hbar/2m)F\left(\psi(r,\theta)/\sqrt{\hbar/2m}\right) \\ &+ \left(\frac{\hbar}{2m}\right)^{1/2} f(r,\theta,h/2m)F'\left(\psi(r,\theta)/\sqrt{\hbar/2m}\right) \\ &+ k(r,\theta,\hbar/2m). \end{aligned} \tag{4.17}$$

In (4.17), g, f and ψ are defined as above, $k(r,\theta,\hbar/2m)$ is the regular perturbation expansion

$$k(r,\theta,h/2m) = \sum_n k^n(r,\theta)\ (\hbar/2m)^n, \tag{4.18}$$

and $F(Z)$ is a special function that satifies (8)

$$\frac{d^2F}{dZ^2} = -Z\,\frac{dF}{dZ} - 1. \tag{4.19}$$

Proceeding as above, we find that ψ, g^0 and f^0 satisfy (4.8), (4.9) and (4.10) respectively and that k^0 satisfies

$$b^r k_r^0 + b^\theta k_\theta^0 - \frac{g^0}{2}\left[\psi_r^2 + \psi_\theta^2\right] = -1. \tag{4.20}$$

The constructions given for $\psi(r,\theta)$ and f^0 above can be used here. The value of g^0, a constant, is determined by evaluating (4.20) on the limit cycle:

$$\frac{g^0}{2}\left[\psi_r^2(r_c)\right] = 1 \tag{4.21}$$

i.e.

$$g^0 = 2/\psi_r^2(r_c). \tag{4.22}$$

Once g^0 is known, k^0 can be calculated by the method of characteristics (9), with initial data $k^0(r,\theta) = 0$ on $r = r_x$. If $\psi(r,\theta) = \bar{\psi}$ on $r = r_x$, we set

$$F(\bar{\psi}/\sqrt{h/2m}) = F'(\bar{\psi}/\sqrt{h/2m}) = 0. \tag{4.23}$$

when integrating (4.19). With this choice of k^0 and $\bar{\psi}$, $T(r,\theta) \equiv 0$ on $r = r_x$. Higher order terms can be treated in an analogous fashion.

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