the details of this experiment or time-dilation effects. The relativistic rotating disk is in any case a much studied topic.[14]

We adopt the *hypothesis that if two bodies in close proximity are relatively at rest for a time, however short, then one can find experimentally if heat passes between them or not.* If this can be applied to the annuli of the two disks, then the possibility of thermal equilibrium for the appropriate portions of the two annuli occurs by (2) and (4) only if $T_1(0) = T_2(0)$. But the ω values can be different, the appropriate radii being given by (4). Would experiment confirm that $T_1(0) = T_2(0)$, and that for given $\omega_1 r_1 \equiv v$, equilibrium with the second annulus occurs at radii r_2 given by $\omega_2 r_2 = v$? To accelerate bodies, large enough to have a temperature, to high velocities presents formidable obstacles. However, we shall assume that it can be done and that (2) is thus confirmed. We have already presented reasons why Eq. (2) is a reasonable formula in any case.

Step 2: A special relativistic experiment is to shoot a small body B with constant velocity

$$v = \omega_1 r_1 \tag{5}$$

in a plane parallel to, but close to, disk A with impact parameter r_1 in such a way that it is instantaneously at rest with respect to the annulus of radius r_1 as it passes just above it. Let the rest temperature of B be $t(0)$. One then has four independent parameters $T_1(0)$, $t(0)$, ω_1, and r_1. This experiment is of even greater difficulty than the last. However, adopting the above *hypothesis*, one may one day be able to find sets of values for which the annulus is in thermal equilibrium with B when the two are in close proximity. If relation (1) holds, the value of a can be determined as follows:

$$T_1(r_1) = t(v) \tag{6}$$

implies $\gamma_1(r_1) T_1(0) = \gamma(\omega_1 r_1)^a t(0)$, whence by (5)

$$a = 1 + \frac{\log[T_1(0)/t(0)]}{\log\gamma(\omega_1 r_1)}. \tag{7}$$

If (7) does not always give the same value of a, then an empirical determination of the temperature transformation is still in principle available from (6) $t(v) = \gamma_1(r) T_1(0)$.

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Classical Quantization of a Hamiltonian with Ergodic Behavior

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Conservative Hamiltonian systems with two degrees of freedom are discussed where a typical trajectory fills the whole surface of constant energy. The trace of the quantum mechanical Green's function is approximated by a sum over classical periodic orbits. This leads directly to Selberg's trace formula for the motion of a particle on a surface of constant negative curvature, and, when applied to the anisotropic Kepler problem, yields excellent results for all the energy levels.

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The relations between classical and quantal mechanics are of central importance to the understanding of physics. Classical mechanics is believed to be a limit of quantum mechanics when Planck's constant is small. It is natural to use the classical motion as a starting point in order

to find an approximate solution for Schrödinger's equation. This idea was implicit in the "old quantum mechanics" of Bohr and Sommerfeld, and was made explicit in the WKB approximation. The latter can be applied to problems with several degrees of freedom provided the separation of variables can be carried out. There are two basic difficulties. First, conserved quantities beyond the energy have to be found which would permit the separation of variables, even if they are not analytic functions of momentum and position. Second, if there are not any, the whole basis for the quantization conditions of Bohr and Sommerfeld vanishes.

The first point was clearly understood by Poincaré and became a frequent topic of investigation by both mathematicians and astronomers in the 1950's. The second point was first discussed by Einstein[1] in 1917 and has received very little attention. The emphasis seems mostly on how to handle the occurrence of nonanalytic constants of motion. Einstein gave the clue when he pointed to the existence of invariant tori on the surface of constant energy in phase space, and he showed the way to the proper treatment of the quantization conditions. But he then goes on to ask how to proceed when there are no invariant tori, not even nearby.

This Letter has two purposes. First, a large class of examples without invariant tori will be shown where a direct connection exists between energy levels and classical orbits. The relevant formula was given by Selberg[2] in 1954 and coincides with a formula which the author[3] proposed some ten years ago for Hamiltonian systems in general. Second, an entirely different example without invariant tori, the anisotropic Kepler problem,[3] will be treated. The same formula gives very close agreement for the energy levels between the solutions of Schrödinger's equation and a method which is based entirely on classical mechanics. Only conservative Hamiltonian systems with two degrees of freedom will be discussed where the typical trajectory (with the exception of a set of measure zero) comes arbitrarily close to every point on the surface of constant energy in phase space. The exceptional set is formed by the closed orbits of which there are many. They are all linearly unstable, i.e., a trajectory which starts nearby in phase space drifts away exponentially fast.

Call $G(q''q'E)$ the quantum mechanical Green's function for such a system (positions q' and q'' with energy E), and write it as a Feymann path integral.[4] The limit $\tilde{G}(q''q'E)$ of $G(q''q'E)$ as Planck's constant $\hbar$ becomes small, is a sum over all classical trajectories from q' to q'' at the energy E. The energy levels can be obtained from the "response functions" $g(E)=\int dq\, G(qqE)$ or $\tilde{g}(E)=\int dq\, \tilde{G}(qqE)$. They exist in a complex E plane and their singularities give the energy levels. $g(E)$ has poles on the real axis, while $\tilde{g}(E)$ may have a more complicated structure which will be interpreted, however, as approximating $g(E)$. All the classical periodic (closed) orbits at the energy E have to be found along with the following quantities: the action integral $S=\oint p\, dq$, the length T_0 (measured in time) of the projection into position space, the number ν of conjugate points, and the stability exponent α. The expression

$$\tilde{g}(E)=-\frac{i}{\hbar}\sum_{\text{per. orb.}}\frac{T_0}{2\sinh\frac{1}{2}\alpha}\exp\left(\frac{i}{\hbar}S-i\nu\frac{\pi}{2}\right) \quad (1)$$

was derived by the author along with a similar formula for systems with invariant tori. In the latter cases, the quantization conditions of Bohr and Sommerfeld were shown to follow immediately.[5]

Selberg's trace formula states that $\tilde{g}(E)=g(E)$, i.e., the approximate expression (1) happens to be exact for a particle moving freely on a surface of constant negative curvature. In Poincaré's model[6] of hyperbolic (Lobachevski) space as the upper Euclidean half-plane $y>0$ with the metric $ds^2=(dx^2+dy^2)/y^2$, a closed surface of constant negative curvature becomes a hyperbolic polygon, i.e., a domain whose boundaries are Euclidean circles with their centers on the x axis and where points on opposite sides are properly identified. A particle moves along a geodesic with constant velocity and its energy E equals its kinetic energy so that $E>0$. The geodesics are again Euclidean circles with their centers on the x axis, but when such a geodesic hits a boundary of the polygon, it has to be continued on the opposite side at the appropriate point with the same direction. The enumeration of the periodic geodesics is difficult to carry out in practice.

With L being the length of the closed geodesic, m being the mass of the particle, and the radius of curvature of the space $R=1$, $S=L(2mE-\hbar^2/4R^2)^{1/2}$. The time T_0 is the simple period, i.e., a submultiple of the total period T, and is given by $T_0=mL_0(2mE-\hbar^2/4R^2)^{-1/2}$ in terms of the simple length L_0. There are no conjugate points, and the stability exponent α equals L. Schrödinger's equation is $\Delta\varphi+\lambda\varphi=0$ with $\lambda=2mE/\hbar^2$ and

periodic boundary conditions corresponding to the identification of opposite sides. The Laplacian Δ is $y^2(\partial^2/\partial x^2+\partial^2/\partial y^2)$ in the Poincaré metric and

$$g(E)=\sum_{n=0}^{\infty}\frac{1}{E-E_n}\ \text{with}\ E_n=\frac{\hbar^2}{2m}\lambda_n, \tag{2}$$

where λ_n is the nth eigenvalue, $\lambda_0=0$. If $\hbar^{-1}(2mE-\hbar^2/4)^{1/2}=i(s-\frac{1}{2})$ and $\mathrm{Re}(s)>\frac{1}{2}$, one finds Selberg's trace formula[7] upon setting $g(E)$ from (2) equal to $\tilde{g}(E)$ from (1),

$$(2s-1)\sum_{n=0}^{\infty}\left(\frac{1}{s(s-1)+\lambda_n}-\frac{1}{s+n}\right)=\sum_{\text{per. orb.}}\frac{L_0}{1-\exp(-L)}e^{-sL}. \tag{3}$$

The term $1/(s+n)$ on the left-hand side comes from the geodesics of zero length (going from q to q) in G and $\tilde{G}$. If it were not so difficult to enumerate the periodic orbits, this formula could be used to determine the spectrum of the Laplacian.

The Hamiltonian of the anisotropic Kepler problem[8] has a kinetic energy with a large mass m_1 in the x direction and a small mass m_2 in the y and z directions, but an ordinary Coulomb potential. If properly normalized,

$$H=\frac{u^2}{2\mu}+\frac{v^2+w^2}{2\nu}-\frac{1}{(x^2+y^2+z^2)^{1/2}} \tag{4}$$

in terms of the position (x,y,z) and the momentum (u,v,w), where $\mu=(m_1/m_2)^{1/2}$ and $\nu=(m_2/m_1)^{1/2}$. The energy E can be used as a scaling parameter. All calculations can be limited to $H=-\frac{1}{2}$. So that for bound states $(E<0)$

$$S=\left(\frac{m_0e^4}{-2\kappa^2E}\right)^{1/2}\oint(udx+vdy+wdz), \tag{5}$$

where the integral is independent of E. For an electron around a donor impurity in silicon, $m_0=(m_1m_2)^{1/2}=0.4177$ electron mass, e is the electron charge, and $\kappa=11.4$ is the dielectric constant.

The angular momentum around the x axis is set to 0. The classical motion can then be limited to the (x,y) plane where the trajectories are inside the circle $x^2+y^2=4$. Each trajectory is started at $t=0$ on the x axis with the initial position x_0 and initial momentum (u_0,v_0), where $v_0>0$. The other intersections with the x axis determine a sequence of reals $(\ldots,x_{-1},x_0,x_1,x_2,\ldots)$ and a binary sequence $(\ldots,a_{-1},a_0,a_1,a_2,\ldots)$ where $a_i=\mathrm{sgn}(x_i)$. To each binary sequence with a period of even length $2n$ corresponds exactly one periodic orbit which closes itself smoothly after crossing the x axis $2n$ times, and vice versa.

The numerical analysis of all such orbits for $n\leq 5$ was made with $\mu^2=4.0$ and $\mu^2=5.0$.[9] The dependence of $\Phi=\oint(udx+vdy)$ on the periodic orbit, is in excellent (but not exact) agreement with the expression

$$\Phi=2n\tau\cosh^2(\tfrac{1}{2}\gamma)-\tfrac{1}{2}\tau\sinh\gamma\sum_{i=1}^{2n}\sum_{j=-\infty}^{+\infty}a_ia_j\exp(-\gamma|j-i|). \tag{6}$$

The parameters γ and τ are chosen such as to give the correct maximum $2n\tau$, and the correct average $n\tau(1+e^{-\gamma})$ in the limit as $n\to\infty$. The minimum is always 0. The mean square deviation of the values (6) from the computed values for $\mu^2=5.0$ and $n=5$ is less than 0.21 while the average of Φ is 22.16. For silicon, $\mu^2=4.80$, $\gamma=0.622$, and $\tau=2.8844$. The crudest approximation was used for α where $\alpha=n\beta$ with $\beta\sim 1.5$. Thus, at least the variations of the action integral from one periodic orbit to another are correctly represented, and may be expected to show the constructive interference in (1) which yields the energy levels. Because of $T=dS/dE$ the period T differs from S only by a factor $\frac{1}{2}E$. The factor T_0 in (1) differs from T in certain cases where the orbit has special symmetries. The correct value of T_0 is obtained if the summation in (1) is carried over all binary sequences of even length $2n$ and T_0 is always replaced by T/n. This rule is independent of the approximation (6). Finally, the number of conjugate points always equals $4n$, exactly as in the ordinary Kepler problem in three dimensions.

When E increases from $-\infty$ to 0 along the real axis, $s=-i(-m_0e^4/2\kappa^2\hbar^2E)^{1/2}$ goes down along the negative imaginary axis starting at the origin, and

$$\int^E\tilde{g}(E)\,dE=\sum_{\text{binary seq.}}\frac{1}{n}\frac{1}{2\sinh\frac{1}{2}\alpha}\exp(-s\Phi). \tag{7}$$

The values of α are quite large, and $2\sinh\frac{1}{2}\alpha$ is replaced by $\exp(\alpha/2)$ (cf. Miller[10]). Some singularities may be lost thereby which are at some distance from the real E axis, and do not yield any sharply defined energy levels.

The expression (7) becomes the grand canonical

partition function of an Ising chain whose two-body exchange interactions decay exponentially with distance. Such systems were treated by Kac[11] in the limit of long-range interaction, i.e., when $\gamma \to 0$. The method of Kac proves very effective in the present situation where γ is not particularly small. The summation over the binary sequences of fixed length $2n$ is transformed into a $2n$-fold integral which can be interpreted as calculating the trace for the $2n$th power of an operator $K(s)$. This operator can be represented as a matrix with reference to the eigenfunctions of the harmonic oscillator. The matrix elements are polynomials in the variable $z = s\tau \sinh\gamma$ apart from an overall factor $2\exp[-s\tau(1+e^{-\gamma})/2]$. The even (odd) harmonic oscillator functions give rise to the energy levels of even (odd) parity.

If $s = 0$, the matrix is diagonal and the eigenvalues are $\exp(-l\gamma)$, with $l = 0, 1, 2, \ldots$. When s moves down along the negative imaginary axis, the eigenvalues $\mu_l(z)$ become complex and spiral clockwise toward the origin. Since only the eigenvalues near the origin contribute potential singularities in (7), it was not necessary to go beyond 50-by-50 matrices, and standard routines for diagonalization:

$$\int^{E} \tilde{g}(E)\,dE = \sum_{l=0}^{\infty} \ln\left[1 - 4\mu_l{}^2(z)\exp\left(-\frac{2z}{e^{\gamma}-1} - \frac{\beta}{2}\right)\right]. \quad (8)$$

where $\mu_l(z)$ depends only on γ. The parameters s and τ occur only in the combination $z = s\tau \sinh\gamma$. If one takes the exponential on both sides, one obtains an infinite product whose logarithmic derivative with respect to E is the response function $\tilde{g}(E)$ and whose zeros are the poles of $\tilde{g}(E)$ just like a good zeta function. With $z = -i\zeta$ (where $\zeta > 0$) starting at 0, the logarithm of $\mu_l(z)$ eventually settles down with a negative real part around -0.3. Therefore, the singularities of (8) occur very near the imaginary z axis, and the resulting energy levels are sharp in spite of the large instability of the individual periodic orbits. The energy levels are given by $E = -m_0 e^4 \tau^2 \sinh^2\gamma / 2\kappa^2\hbar^2\zeta^2$, where ζ is such that the phase of $2\mu_l \times \exp(\,)$ in (8) is an odd multiple of π.

The resulting values of E for silicon are compared in Table I with those of Faulkner[12] who solved Schrödinger's equation by the variational method using a basis set of hydrogenlike functions with principal quantum numbers 1 through 5 for even parity and 2 through 6 for odd parity. The designation of the energy levels is identical with that of the author's earlier results in Ref. 3. These were based on the knowledge of only the simplest periodic orbit, $(+-)$ of length 2 and $\Phi = 2\tau$, and were only meant as a crude trial. There is clearly a vast improvement both in the accuracy of the numbers and the completeness of the results.

TABLE I. Energy levels for a donor impurity in silicon. Designation of the levels in columns 1 and 5, earlier results in columns 2 and 6, results of the present work in columns 3 and 7, Faulkner's results in columns 4 and 8. Units are millielectronvolts.

	Even parity				Odd parity		
1*s*	36.81	29.06	31.27	2*p*	9.20	10.48	11.51
2*s*		8.35	8.83	3*p*		5.10	5.48
3*d*	4.09	4.63	4.75	4*p*		3.12	3.33
3*s*		3.64	3.75	4*f*	2.30	2.30	2.33
4*d*		2.82	2.85	5*p*		2.15	2.23
4*s*		2.11	2.11	5*f*		1.64	1.62
5*d*		1.87	1.87	6*p*		1.49	1.52
5*g*	1.47	1.53	1.52	6*f*		1.32	1.20
5*s*		1.43	1.38	6*h*	1.02	1.09	1.10

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