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$$\psi(\boldsymbol{r}, t) \underset{r\to\infty}{\simeq} \int_0^\infty \mathrm{d}k\, f(k) \mathrm{e}^{\mathrm{i}kz} \exp(-\mathrm{i}E(k)t/\hbar)$$
$$+ \int_0^\infty \mathrm{d}k\, f(k) F_k(\theta, \varphi) \frac{\mathrm{e}^{\mathrm{i}kr}}{r} \exp(-\mathrm{i}E(k)t/\hbar). \quad (62)$$

Although the second one is not exactly of the form studied above, they can both be treated by the stationary-phase method (§2.1.2). The central position of the first packet is then found at

$$z_{\mathrm{p}}(t) = \frac{\hbar k_0}{m} t \qquad x_{\mathrm{p}} = y_{\mathrm{p}} = 0. \quad (63)$$

As for the scattered wave packet, the location of its maximum depends on the direction (θ, φ) chosen; the distance between this maximum and the origin of the coordinate system is given by

$$r_{\mathrm{s}}(\theta, \varphi; t) = -\delta'_{k_0}(\theta, \varphi) + \frac{\hbar k_0}{m} t \quad (64)$$

where $\delta'_k(\theta, \varphi)$ is the derivative with respect to k of the phase of the scattering amplitude $F_k(\theta, \varphi)$. These formulae are valid only in the asymptotic region (that is, for large $|t|$). Their discussion goes along the same lines as above. *For large negative values of t, there is no scattered wave packet*: the waves that build it interfere constructively only for negative values of r and these are, of course, not permitted. Therefore, all that is found long before the collision is the *plane wave packet* which is then to be identified with the *incident wave packet. For large positive values of t, both packets are effectively present*: the first one continues along the path of the incident packet and the second one diverges in all directions. *The scattering cross section can then be deduced from the consideration of these wave packets.* (Actually, one should also allow for slightly different orientations of the incident wavevector $\boldsymbol{k}$, in order to limit the plane wave packet not only along 0z, but also in the perpendicular directions.) Here too, *the same result can be obtained much more simply using the 'probability fluid'* and the corresponding 'improper interpretation' of a stationary state (Cohen-Tannoudji *et al* 1977, p 912).

So the questions raised and arguments discussed in the present paper can actually be applied to a much wider domain than just the one-dimensional square potential problems.

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Exact Aharonov–Bohm wavefunction obtained by applying Dirac's magnetic phase factor

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Abstract A solution of Schrödinger's equation for a particle in a magnetic field $\boldsymbol{B}$ can be obtained from the wavefunction when $\boldsymbol{B} = 0$ by Dirac's prescription of multiplication by a phase factor. But this solution is often multiple-valued and hence unsatisfactory. It is shown that in the case of the Aharonov–Bohm effect the Dirac prescription can nevertheless be made to yield the single-valued exact wavefunction, provided it is applied not to the total wave with $\boldsymbol{B} = 0$ but to its separate components in a 'whirling-wave' representation. The mth whirling wave at a point $\boldsymbol{r}$ is a contribution that has arrived at $\boldsymbol{r}$ after travelling m times around the region containing $\boldsymbol{B}$.

Résumé On peut obtenir une solution de l'équation de Schrödinger pour une particule placée dans un champ magnétique $\boldsymbol{B}$, à partir de la solution en champ nul, en appliquant la prescription de Dirac de multiplication par un facteur de phase. Mais cette solution est souvent multiforme et, par suite, non satisfaisante. On montre ici que, dans le cas de l'effet Aharonov–Bohm, on peut néanmoins tirer de la prescription de Dirac la fonction d'onde exacte, (et uniforme); mais il faut pour cela appliquer cette prescription, non pas à l'intégralité de la fonction d'onde en champ nul, mais, séparément, à ses diverses composantes dans une représentation où la $m^{\text{ème}}$ composante en $\boldsymbol{r}$ correspond à la contribution qui est parvenue au point $\boldsymbol{r}$ après avoir tourné m fois autour de la région où se manifeste le champ $\boldsymbol{B}$.

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1 Dirac's prescription

This article is about the quantum mechanics of a particle in the presence of a magnetic field $\boldsymbol{B}$, which will be represented by a vector potential $\mathbf{A}$. This must satisfy

$$\oint \mathbf{A} \cdot \mathrm{d}\boldsymbol{r} = \int\int \boldsymbol{B} \cdot \mathrm{d}\boldsymbol{S} \tag{1}$$

where the first integral is around any closed curve C and the second is over any surface bounded by C. Locally, (1) implies

$$\boldsymbol{B} = \nabla \wedge \mathbf{A}. \tag{2}$$

Then as is well known the Hamiltonian operator describing the particle is

$$H(\boldsymbol{r}, \boldsymbol{p}) = H_0(\boldsymbol{r}, \boldsymbol{p} - q\mathbf{A}) \tag{3}$$

where $H_0(\boldsymbol{r}, \boldsymbol{p})$ is the Hamiltonian without the magnetic field but with all other forces unaltered, q is the charge on the particle and, working in position representation, $\boldsymbol{p}$ is the momentum operator $-i\hbar\nabla$. I shall consider wavefunctions $\psi(\boldsymbol{r})$ corresponding to particles with fixed energy E, which must therefore satisfy Schrödinger's equation

$$H(\boldsymbol{r}, -i\hbar\nabla)\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r}). \tag{4}$$

As pointed out by Dirac (1931), a function $\psi_{\mathrm{D}}(\boldsymbol{r})$ satisfying (4) can be constructed very simply, in terms of the wave in the absence of the field, i.e. in terms of $\psi_0(\boldsymbol{r})$ which satisfies

$$H_0(\boldsymbol{r}, -i\hbar\nabla)\psi_0(\boldsymbol{r}) = E\psi_0(\boldsymbol{r}). \tag{5}$$

The construction consists in multiplying ψ_0 by a 'magnetic phase factor' as follows:

$$\psi_{\mathrm{D}}(\boldsymbol{r}) = \psi_0(\boldsymbol{r}) \exp\left(\frac{iq}{\hbar}\int_{\boldsymbol{r}_0}^{\boldsymbol{r}} \mathbf{A}(\boldsymbol{r}') \cdot \mathrm{d}\boldsymbol{r}'\right) \tag{6}$$

where $\boldsymbol{r}_0$ is an arbitrary fixed position.

The trouble with Dirac's prescription is that although ψ_{D} satisfies the wave equation (4) it is not single-valued and therefore cannot correctly represent the true quantum state in the presence of $\boldsymbol{B}$. To see why (6) is multivalued, let $\boldsymbol{r}$ be transported round a loop C back to the same point. During this process, the phase of (6) changes by

$$\Delta_{\mathrm{C}}\chi = \frac{q}{\hbar}\oint_{\mathrm{C}} \mathbf{A} \cdot \mathrm{d}\boldsymbol{r} = \frac{q}{\hbar}\Phi_{\mathrm{C}} \tag{7}$$

where according to (1) Φ_{C} is the flux of $\boldsymbol{B}$ through C. As well as being multivalued, ψ_{D} would, if it really represented the state, imply that the magnetic field has no effect on the probability density $|\psi|^2$, which is obviously not the case.

Despite these difficulties, Dirac's prescription has been used in an inexact way to make predictions about the effect of a magnetic field, and these have been experimentally verified. In this inexact procedure, it is imagined that $\psi_0(\boldsymbol{r})$ consists of two parts, written as

$$\psi_0(\boldsymbol{r}) = \psi_0^{(1)}(\boldsymbol{r}) + \psi_0^{(2)}(\boldsymbol{r}), \tag{8}$$

corresponding to waves reaching $\boldsymbol{r}$ by different routes labelled 1 and 2. The effect of $\boldsymbol{B}$ is then included by incorporating the magnetic phase factor (6) into each part separately. This gives

$$\begin{aligned}\psi_{\mathrm{D}}(\boldsymbol{r}) &= \psi_0^{(1)}(\boldsymbol{r}) \exp\left(\frac{iq}{\hbar}\int_{\substack{\boldsymbol{r}_0\\ \text{path 1}}}^{\boldsymbol{r}} \mathbf{A} \cdot \mathrm{d}\boldsymbol{r}\right) + \psi_0^{(2)}(\boldsymbol{r}) \exp\left(\frac{iq}{\hbar}\int_{\substack{\boldsymbol{r}_0\\ \text{path 2}}}^{\boldsymbol{r}} \mathbf{A} \cdot \mathrm{d}\boldsymbol{r}\right)\\ &= \exp\left(\frac{iq}{\hbar}\int_{\substack{\boldsymbol{r}_0\\ \text{path 1}}}^{\boldsymbol{r}} \mathbf{A} \cdot \mathrm{d}\boldsymbol{r}\right) \times \left[\psi_0^{(1)}(\boldsymbol{r}) + \psi_0^{(2)}(\boldsymbol{r}) \exp\left(\frac{iq\Phi}{\hbar}\right)\right]\end{aligned} \tag{9}$$

where Φ is the flux through the loop from $\boldsymbol{r}_0$ to $\boldsymbol{r}$ along path 2 and back to $\boldsymbol{r}$ along path 1. In physical terms, this result predicts a change in the interference between $\psi_0^{(1)}$ and $\psi_0^{(2)}$ because their relative phase has been changed by the factor involving Φ. But the exponential prefactor remains, and will still cause ψ_{D} to be multivalued and hence unsatisfactory.

My purpose here is to show, using the example of the Aharonov–Bohm effect, how Dirac's prescription can in fact be used to obtain the exact wavefunction in the presence of a field. The procedure will be to decompose ψ_0, which of course is single-valued, into an infinite number of components ('whirling waves'), each of which is multivalued, then to apply (6) to each whirling wave, and finally to resum the magnetically phase-shifted whirling waves to get the exact single-valued wavefunction ψ.

2 Aharonov–Bohm effect for thin solenoids

Aharonov and Bohm (1959) considered a field $\boldsymbol{B}$ confined within a long straight solenoid directed along the z axis and containing flux Φ. Charged particles with energy E and mass m are incident from the positive x direction (figure 1). They are scattered by the solenoid but cannot penetrate into it. Aharonov and Bohm came to the surprising conclusion (which is still controversial—see Casati and Guarneri (1979), Roy (1980) and the remarks at the end of the paper by Berry *et al* (1980)) that the flux Φ can affect particles even though the region containing the field is inaccessible to the particles. This comes about because the Hamiltonian (3) involves Φ not through its field $\boldsymbol{B}$ but through the vector potential $\mathbf{A}$, which, because of (1), cannot vanish outside the solenoid, since its line integral must equal Φ. I shall use the simplest potential satisfying this condition, namely

$$\mathbf{A}(\boldsymbol{r}) = \frac{\Phi}{2\pi r}\hat{\boldsymbol{\theta}} \tag{10}$$

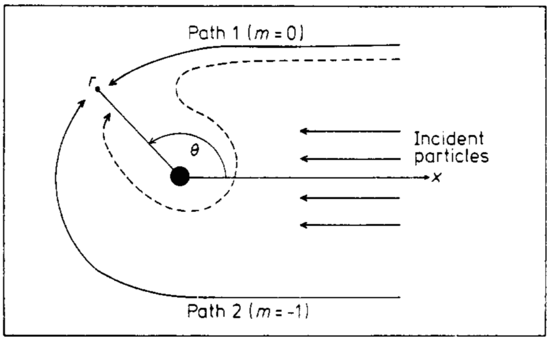

Figure 1 Geometry of the Aharonov–Bohm effect. The solenoid is shown in cross section as a black circle and carries flux of a magnetic field normal to the page. Two paths reaching a point $\boldsymbol{r}$ are shown; the broken path is equivalent to path 2.

where $r, \hat{\theta}$ are plane polar coordinates and $\hat{\boldsymbol{\theta}}$ is the azimuthal unit vector.

In the simplest case, the solenoid is idealised as being infinitely thin, so that we are considering scattering by a single flux line. The incident beam has the wavefunction

$$\psi_0(\boldsymbol{r}) = \exp(-\mathrm{i}kx) = \exp(-\mathrm{i}kr\cos\theta) \qquad (11)$$

where

$$k = \sqrt{2mE}/\hbar. \qquad (12)$$

We seek the wave ψ when Φ is non-zero. This must satisfy the 'inpenetrability' condition that $\psi = 0$ on the flux line at $r = 0$.

Consider first the Dirac prescription (6). With $\boldsymbol{r}_0$ taken at a point on the positive x axis this involves the phase

$$\frac{q}{\hbar}\int_{r_0}^{r} \mathbf{A}(\boldsymbol{r}')\cdot \mathrm{d}\boldsymbol{r}' = \frac{q\Phi}{h}\int_0^\theta \frac{1}{r}\hat{\boldsymbol{\theta}}'\cdot \mathrm{d}\boldsymbol{r}' = \alpha\theta \qquad (13)$$

where α is the magnetic flux parameter, defined by

$$\alpha \equiv q\Phi/h. \qquad (14)$$

Therefore (6) converts (11) into the magnetically phase-shifted wave

$$\psi_{\mathrm{D}}(\boldsymbol{r}) = \exp(-\mathrm{i}kr\cos\theta + \mathrm{i}\alpha\theta). \qquad (15)$$

The multivaluedness is now explicit: ψ_{D} changes by a factor $\exp(2\pi\mathrm{i}\alpha)$ during a circuit of the solenoid, and this factor is not unity unless α is an integer, i.e. unless the flux is quantised. Moreover, ψ_{D} does not vanish at $r = 0$.

3 Poisson transformation to whirling waves

In obtaining the exact solution ψ from the solution (11) without the field, the first step is to express ψ_0 as an angular momentum decomposition into partial waves by making use of the relation (Gradshteyn and Ryzhik 1965)

$$\exp(-\mathrm{i}kr\cos\theta) = \sum_{l=-\infty}^{\infty} (-\mathrm{i})^{|l|} J_{|l|}(kr)\exp(\mathrm{i}l\theta). \qquad (16)$$

The modulus signs on two of the l indices do not affect the value of the sum but are nevertheless important for a reason soon to be explained.

Next, we transform the summation over l by means of the Poisson summation formula (Lighthill 1958). For any summand $F(l)$, this replaces the sum by a series of integrals over $F(\lambda)$ which is any 'interpolation' of $F(l)$ to non-integral values of its variable. The formula is

$$\sum_{l=-\infty}^{\infty} F(l) = \sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}\lambda\, F(\lambda)\exp(2\pi\mathrm{i}m\lambda). \qquad (17)$$

When applied to (16) it gives

$$\psi_0(r,\theta) = \sum_{m=-\infty}^{\infty} T_m(r,\theta) \qquad (18)$$

where

$$T_m(r,\theta) \equiv \int_{-\infty}^{\infty} \mathrm{d}\lambda\, \exp(-\tfrac{1}{2}\mathrm{i}\pi|\lambda|) J_{|\lambda|}(kr) \times \exp[\mathrm{i}\lambda(\theta + 2\pi m)]. \qquad (19)$$

The terms T_m are not single-valued. In fact

$$T_m(r,\theta + 2\pi) = T_{m+1}(\boldsymbol{r},\theta) \qquad (20)$$

as follows easily from (19). It is this relation that ensures the single-valuedness of the sum (18) despite the multivaluedness of its terms.

Now comes the most important step, which consists of an interpretation of T_m based on the fact that these terms contain θ in the combination $\theta + 2\pi m$. This is to restrict θ by $-\pi < \theta \leqslant +\pi$ and then interpret $T_m(r,\theta)$ as *a wave arriving at θ after making m anticlockwise circuits of the origin.* I shall call $T_m(r,\theta)$ the mth 'whirling-wave' component of ψ_0. Each whirling wave is a (multivalued) solution of Schrödinger's equation without the magnetic flux. Therefore, Dirac's prescription (6) can be applied to yield a whirling wave satisfying Schrödinger's equation in the presence of the flux. The phase is given by (13), but instead of θ we must write $\theta + 2\pi m$ because that is the total angle turned through. The new whirling waves are therefore

$$T_m^{\mathrm{D}}(r,\theta) = T_m(r,\theta)\exp[\mathrm{i}\alpha(\theta + 2\pi m)]. \qquad (21)$$

Summing over m gives, on using (19), the wave

$$\psi(r,\theta) = \sum_{m=-\infty}^{\infty} T_m^{\mathrm{D}}(r,\theta) = \sum_{m=-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}\lambda\, \exp(-\tfrac{1}{2}\mathrm{i}\pi|\lambda|) J_{|\lambda|}(kr) \times \exp[\mathrm{i}(\lambda + \alpha)(\theta + 2\pi m)]. \qquad (22)$$

On defining $\lambda+\alpha$ as a new variable this can be reverse-Poisson-transformed to give

$$\psi(r,\theta)=\sum_{l=-\infty}^{\infty}(-\mathrm{i})^{|l-\alpha|}J_{|l-\alpha|}(kr)\exp(\mathrm{i}l\theta). \quad (23)$$

The wave (23) satisfies Schrödinger's equation and is manifestly single-valued. In fact it is the exact solution of the problem originally obtained by Aharonov and Bohm (1959), who used a quite different procedure. When the flux is quantised, i.e. when α is an integer, (23) reduces simply to the incident wave (11) multiplied by a phase factor $\exp(\mathrm{i}\alpha\theta)$ which is single-valued. When α is not an integer, (23) contains a wave scattered out towards $r=\infty$ by the flux line, as well as a complicated phase structure centred on the flux line; since both these aspects of the Aharonov–Bohm wavefunction have been recently discussed by Berry *et al* (1980), I shall not dwell on them further here, except to make one point. This is that for non-integral α, when the flux has a physical effect on the wave, ψ as given by (23) vanishes as $r\to 0$, showing that the wave is indeed zero where the flux is non-zero. If the modulus signs had not been inserted into the original summation (16), this result would not have been obtained, and indeed the integrals (19) for the individual whirling waves would have diverged.

4 Generalisation and discussion

Now let the solenoid be of finite radius. This can be modelled by a cylindrically symmetric scalar potential field with a 'hard core' at a finite radius, preventing the particles from entering the region where the flux is. The wave ψ_0 in the absence of the flux is now not just the incident wave (11), but includes the wave scattered by the cylinder. Therefore the partial-wave decomposition of ψ_0 is

$$\psi_0(r,\theta)=\sum_{l=-\infty}^{\infty}R_{|l|}(r)\exp(\mathrm{i}l\theta) \quad (24)$$

where $R_{|l|}(r)$ is the solution of the radial equation with angular momentum (l) obtained by separation of the variables r and θ in the two-dimensional Schrödinger equation obtained from (5) and including a repulsive potential excluding particles from the cylinder.

Again the Poisson formula (17) can be employed to transform the sum over l, with the result that ψ_0 is given by (18) with T_m defined by

$$T_m(r,\theta)=\int_{-\infty}^{\infty}\mathrm{d}\lambda\, R_{|\lambda|}(r)\exp[\mathrm{i}\lambda(\theta+2\pi m)] \quad (25)$$

instead of (19). And again the $T_m(r,\theta)$ can be regarded as whirling waves and magnetically phase-shifted as in (21), to give the wave ψ scattered by a finite cylinder containing flux Φ:

$$\psi(r,\theta)=\sum_{m=-\infty}^{\infty}T_m(r,\theta)\exp[\mathrm{i}\alpha(\theta+2\pi m)]. \quad (26)$$

This can be reverse-Poisson-transformed to give

$$\psi(r,\theta)=\sum_{l=-\infty}^{\infty}R_{|l-\alpha|}(r)\exp(\mathrm{i}l\theta) \quad (27)$$

which again is the exact solution.

The outcome of this analysis is that it is possible to obtain single-valued wavefunctions by means of the Dirac prescription (6), provided this is applied to the correct representation of the wavefunction in the absence of the field. In the Aharonov–Bohm effect this representation consists of a decomposition into whirling waves T_m. Mathematically, these arise because the impenetrable cylinder makes the space multiply connected, so that paths encircling the origin different numbers of times cannot be deformed into one another and must be given magnetic phase shifts which take account of the different numbers of circuits. It seems likely that the same idea could be employed to solve other problems involving magnetic fields.

We are now in a position to understand why the inexact argument presented in §1 is often successful. Depending on the precise scattering properties of the cylinder, it may be the case that in a particular angular region only two of the whirling waves (25) have appreciable and comparable magnitudes. These may be represented, for example, by the two paths shown in figure 1, which correspond to $m=0$ (path 1) and $m=-1$ (path 2) (to see that path 2 does indeed correspond to $m=-1$, simply note that it can be obtained from path 1 by adding a single clockwise circuit of the cylinder as illustrated by the broken path in figure 1). Then in this angular region we may approximate ψ by

$$\psi_0(r,\theta)\simeq T_0(r,\theta)+T_{-1}(r,\theta) \quad (28)$$

which is precisely of the previously assumed form (8). Applying the Dirac prescription (21) now gives the analogue of (2), namely

$$\psi(r,\theta)=\exp(\mathrm{i}\alpha\theta)[T_0(r,\theta)+\exp(-2\mathrm{i}\pi\alpha)T_{-1}(r,\theta)]. \quad (29)$$

As noted earlier, this is not single-valued. Now we can see why: although the neglected whirling waves ($m\neq 0$ or -1) are small in the angular region considered, they become large when θ increases by 2π (because of (20)) and must be included if ψ is to be single-valued after a circuit of the cylinder.

The whirling waves T_m into which ψ_0 is decomposed are unfamiliar, and I conclude with a brief discussion of them. For a cylinder whose radius is large in comparison with the de Broglie wavelength $2\pi/k$ of the incident wave, it is valid to employ semiclassical methods to obtain an asymptotic approximation for ψ_0. Such analysis is now standard (see e.g. Rubinov 1961, Berry and Mount 1972) and yields the result that the Poisson formula leads to contributing $T_m(r, \theta)$ which can be expressed in terms of *trajectories* arriving at r, θ after encircling the origin m times. If the cylinder is surrounded by a region of attracting potential, some of these trajectories can be actual classical orbits winding smoothly around several times before emerging. Otherwise, they can be 'diffracted rays' (Keller 1958) which skim around the impenetrable surface of the cylinder before emerging tangentially. But I emphasise that the whirling-wave representation is exact and fully quantum mechanical, independent of any semiclassical interpretation. This should be clear from the fact that it was introduced in §3 as a representation of a plane wave without any scatterer, so that the whirling waves are a consequence of choosing a line in space (later to be occupied by a flux line) around which rotations are to be counted, and around which no 'real' rays are winding. In this case formula (19) for the whirling waves can be reduced a little by contour integration:

$$T_m(r, \theta) = \exp(-ikr\cos\theta)\delta_{mo} - \frac{1}{\pi}\int_{-\infty}^{\infty} dy \frac{(\pi + iy)\exp(ikr\cosh y)}{(\pi+iy)^2 - (\theta + 2\pi m)^2} \qquad (-\pi < \theta \leqslant +\pi). \quad (30)$$

The first term in this strange representation is just the original plane wave being decomposed, and winds zero times around the origin. The other term gives zero when summed over m, as it must, and radiates outwards as well as whirling.

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The Wigner function: I. The physical interpretation

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Abstract It is being argued that even in non-relativistic quantum mechanics the coordinate and momentum variables cannot be interpreted directly as observables. Only by defining these by suitable test bodies can we obtain verifiable predictions. When these arguments are implemented on a Wigner distribution we show that positive phase space probabilities always ensue, and hence this function can be used as a quantum mechanical phase space function.

Zusammenfassung Es wird gezeigt, dass auch in der nichtrelativistischen Quantenmechanik die Koordinaten und Impulsvariablen nicht direkt als Observable interpretiert werden können. Nur wenn man diese Grössen durch geeignete Testkörper definiert kann man überprüfbare Vorhersagen erhalten. Die Anwendung dieser Argumente auf eine Wigner'sche Verteilungsfunktion zeigt, dass sich stets positive Wahrscheinlichkeiten im Phasenraum ergeben, und dass diese Funktion daher als Mass für den quantenmechanischen Phasenraum dienen kann.

1 Introduction

The relationship between a quantum mechanical description of particles and its classical counterpart has been the object of much discussion. The standard method to obtain the classical limit (Dirac 1958) makes contact with classical mechanics at one of its least intuitively transparent points, the action principle of higher dynamics. As the Hamilton–Jacobi formalism deals with families of trajectories rather than individual objects, one can easily make a transition to phase space statistical mechanics. On the other hand, quantum mechanics deals with statistical predictions only, and hence it is natural to regard its classical limit to comprise a description in terms of ensembles. The agreement between the classical limit of quantum mechanics and a classical ensemble is an agreement about the

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