A Geometric Picture of the Wave Function: Fermi’s Trick

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Abstract
We show that there is a one-to-one correspondence between wave functions and surfaces in the position-momentum phase plane bounded by a closed curve satisfying an exact quantum condition refining the usual EBK condition. This is achieved using an old forgotten idea of Enrico Fermi.

1 Introduction
We address in this paper the following simple questions:

Given a wave function \( \psi(x) \) defined on the real line, is it possible to give an unambiguous two-dimensional pictorial representation of that function as a surface in position-momentum phase plane? Conversely, under which conditions can one associate to such a surface a wave function?

We will show that there is indeed a one-to-one correspondence between wave functions and surfaces in phase plane whose boundary is a closed curve satisfying a certain quantum condition. Our proof is based on two results, the first of which has almost sunk into oblivion: “Fermi’s trick” \([5]\) which associates to every wave function a curve, and the existence of an exact quantization condition for such curves. More precisely, we will see that:

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Every twice differentiable complex function $\psi$ satisfies a linear (second order) differential equation

$$\left[ \left( -i\hbar \frac{d}{dx} - f(x) \right)^2 + g(x) \right] \psi = 0; \quad (1)$$

Closed phase plane curves

$$p = p^+(x) \geq 0, \quad p = p^-(x) \leq 0 \quad (x_A \leq x \leq x_B) \quad (2)$$

are in one-to-one correspondence with functions $\psi$ provided they satisfy an exact quantization condition [17, 18, 20].

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2 Fermi’s trick

In a largely forgotten paper [5] from 1930 Enrico Fermi shows that one could associate to every quantum state $\psi$ a certain curve $g_F(x, p) = 0$ in phase plane. He remarked that one could explicit determine a second order differential equation satisfied by a twice differentiable complex function. Fermi’s work has recently rediscovered by Benenti and Strini [4, 3]. The underlying idea is actually surprisingly simple. It consists in observing that any complex twice continuously differentiable function $\psi(x) = R(x) e^{iS(x)/\hbar}$ ($R(x) > 0$ and $S(x)$ real) defined on configuration space trivially satisfies the partial differential equation

$$\left( -\hbar^2 \frac{d^2}{dx^2} + \hbar^2 \frac{R''}{R} \right) R = 0 \quad (3)$$

(it is assumed throughout that $R$ satisfies the concavity condition $R'' \leq 0$). Performing the gauge transformation

$$-i\hbar \frac{d}{dx} \rightarrow -i\hbar \frac{d}{dx} - S'$$

this equation is equivalent to

$$\left[ \left( -i\hbar \frac{d}{dx} - S' \right)^2 + \hbar^2 \frac{R''}{R} \right] \psi = 0 \quad (4)$$
(the equivalence of Eqns. 3 and 4 can also be verified by a direct explicit calculation). The operator
\[ \hat{g}_F = \left( -i\hbar \frac{d}{dx} - S' \right)^2 + \hbar^2 \frac{R''}{R} \] appearing in the left-hand side of Eqn. 4 is the quantization of the real function
\[ g_F(x,p) = (p - S')^2 + \hbar^2 \frac{R''}{R} \] and the equation \( g_F(x,p) = 0 \) in general determines a curve \( C_F \) in the phase plane, which Fermi ultimately identifies with the state \( \psi \) itself. Notice that the Fermi function only depends on the state \( \psi \) in the sense that if the replacement of \( \psi \) with \( \lambda \psi \) (\( \lambda \neq 0 \) a complex constant) changes neither \( g_F \) nor \( \hat{g}_F \).

Let us illustrate Fermi’s trick when \( \psi \) is a Gaussian \( \psi_{a,b}(x) = e^{-(a+ib)x^2/2\hbar}. \) In this case we have \( S(x) = -bx^2/2 \) and \( R(x) = e^{-ax^2/2\hbar} \) hence
\[ g_F(x,p) = (p + bx)^2 + ax^2 - \hbar. \]
The Gaussian \( \psi_{a,b} \) is thus a solution of the eigenvalue problem
\[ \frac{1}{2} \left[ \left( -i\hbar \frac{d}{dx} + bx \right)^2 + ax^2 \right] \psi = \frac{1}{2} \hbar \psi. \]
For instance, if \( a = 1 \) and \( b = 0 \) one recovers the fact that the standard Gaussian \( e^{-x^2/2\hbar} \) is the ground state of the harmonic oscillator.

### 3 An exact quantization rule

Consider the one-dimensional stationary Schrödinger equation
\[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) = [E - V(x)]\psi(x). \] We assume that the potential \( V \) is piecewise continuous, and that there exist exactly two real values \( x_A \) and \( x_B \) (“turning points”) such that
\begin{align*}
V(x) > E & \text{ for } -\infty < x < x_A \text{ or } x_B < x < +\infty \\
V(x) = E & \text{ for } x = x_A \text{ or } x = x_B \\
V(x) < E & \text{ for } x_A < x < x_B.
\end{align*}
It follows from elementary functional analysis (Sturm–Liouville theory) that the equation (7) has non-zero solutions only for a set of discrete values $E_0 \leq E_1 \leq \cdots$ of the energy $E$. In [17, 18] Ma and Xu have shown that these values can be explicitly calculated using an exact quantization rule.

The argument goes as follows: let $\chi = \psi' / \psi$ be the logarithmic derivative of the wavefunction $\psi$; a straightforward calculation shows that Schrödinger’s equation (7) is equivalent to the Riccati equations

$$- \chi'(x) = k(x)^2 + \chi(x)^2 \quad \text{for } V(x) \leq E$$
$$- \chi'(x) = -k(x)^2 + \chi(x)^2 \quad \text{for } V(x) \geq E;$$

where $k(x)$ is given by

$$k(x) = \begin{cases} 
\frac{1}{\hbar} \sqrt{2m(E - V(x))} & \text{for } V(x) \leq E \\
\frac{1}{\hbar} \sqrt{2m(V(x) - E)} & \text{for } V(x) \geq E
\end{cases}$$

(8)

(the function $p(x) = \hbar k(x)$ is the momentum). Supposing that the potential $V(x)$ is continuous at the turning points $x_A$ and $x_B$, the exact quantum condition of Ma and Xu is then

$$\int_{x_A}^{x_B} k(x) dx - \int_{x_A}^{x_B} \chi(x)[\chi'(x)]^{-1} k'(x) dx = N\pi$$

(9)

where $N$ is the number of nodes of $\chi$ for $V(x) \leq E$ (hence $N-1$ is the number of nodes of $\psi$ in that region). Notice that if the second integral is neglected, the formula above reduces to the familiar approximate Bohr–Sommerfeld or WKB prescription

$$\int_{x_A}^{x_B} k(x) dx = N\pi.$$ 

(10)

We mention that Barclay [2] had shown in some older and unfortunately rather overlooked work that one can obtain exact quantization rules by a clever re-summation procedure of the higher order terms in the WKB series.

A crucial fact noted by Qian and Dong [20] (also see Serrano et al. [21, 22]) is that condition (9) can be put for all exactly solvable systems in the simple form

$$\int_{x_A}^{x_B} k(x) dx - \int_{x_A}^{x_B} k_0(x) dx = (N - 1)\pi$$

(11)

where the function $k_0$ is defined by (8) with $E = E_0$ (the ground energy level):

$$\hbar k_0(x) = \sqrt{2m(E_0 - V(x))} \quad \text{for } V(x) \leq E.$$ 

(12)
The exact quantization condition thus becomes
\[
\int_{x_A}^{x_B} \sqrt{2m[E - V(x)]} dx = \int_{x_A}^{x_B} \sqrt{2m[E_0 - V(x)]} dx + \frac{Nh}{2} \quad (13)
\]
which shows that the energy levels \(E_1, E_2, \ldots\) are determined by the ground state energy level \(E_0\). Denoting by \(\mathcal{C}\) (resp. \(\mathcal{C}_0\)) the curve
\[
\frac{1}{2m}p^2 + V(x) = E \quad \text{(resp. } \frac{1}{2m}p^2 + V(x) = E_0)\]
this is equivalent to
\[
\int_{\mathcal{C}} p dx = \int_{\mathcal{C}_0} p dx + Nh. \quad (14)
\]
While a general condition for systems with \(n\) degrees of freedom is still lacking, the procedure outlined above still applies to \(n\)-dimensional systems with spherical symmetry in which case \(V(x)\) is replaced by the effective potential \(V_{\text{eff}}(r)\) (see [16, 17, 18, 20]). This allows, in particular, to recover the energy levels of the hydrogen atom.

4 Wave-functions and surfaces in phase plane

4.1 From \(\psi\) to \(\Omega\)

Let \(\psi = Re^{iS/\hbar} (R > 0)\) be a solution of the stationary Schrödinger equation [7]; assume for instance it corresponds to the \(N\)-th energy level \(E_N\). A direct calculation shows that the function \(R\) satisfies the equation
\[
\frac{1}{2m} \left( -i\hbar \frac{d}{dx} - S'(x) \right)^2 R(x) = [E - V(x)]R(x) \quad (15)
\]
and the corresponding Fermi function is thus
\[
g_F(x,p) = (p - S'(x))^2 + 2m(E_N - V(x)). \quad (16)
\]
The area of the surface \(\Omega\) bounded by the curve \(\mathcal{C} : g_F(x,p) = 0\) is given by the formula
\[
\text{Area}(\Omega) = 2 \int_{x_A}^{x_B} \sqrt{2m[E_N - V(x)]} dx.
\]
In view of the quantization condition [13] this means that we have
\[
\text{Area}(\Omega) = Nh + 2 \int_{x_A}^{x_B} \sqrt{2m[E_0 - V(x)]} dx. \quad (17)
\]
Let us illustrate this on the harmonic oscillator with classical Hamiltonian
\[ H = \frac{1}{2m}(p^2 + m^2\omega^2x^2). \]
The ground energy is \( E_0 = \frac{1}{2}\hbar\omega \) and the corresponding turning points are \( \pm \sqrt{\hbar/m\omega} \) hence
\[
\text{Area}(\Omega) = N\hbar + 2\sqrt{m\hbar\omega} \int_{-\sqrt{\hbar/m\omega}}^{\sqrt{\hbar/m\omega}} \sqrt{1 - \frac{m\omega}{\hbar}x^2} dx;
\]
the integral is easily evaluated, and one finds that
\[
\text{Area}(\Omega) = (N + \frac{1}{2})\hbar
\]
and one thus recovers the fact that the action increases by jumps equal to \( \hbar \) starting from the initial value \( \frac{1}{2}\hbar \).

### 4.2 From \( \Omega \) to \( \psi \)

We now address the converse problem. Consider a smooth closed curve \( C \) (see Fig. 1) described by equations
\[
p = p^+(x), \quad p = p^-(x) \quad (x_A \leq x \leq x_B);
\]
with \( p^+(x_A) = p^-(x_A), \quad p^+(x_B) = p^-(x_B) \) and \( p^+(x) \geq 0, \quad p^+(x) \leq 0 \). Defining functions \( f(x) \) and \( g(x) \) through
\[
p^+(x) = f(x) + \sqrt{-g(x)} \quad , \quad p^-(x) = f(x) - \sqrt{-g(x)}
\]
the curve \( C \) is given by the single equation
\[
(p - f(x))^2 + g(x) = 0
\]
and the area of the surface \( \Omega \) enclosed by \( C \) is
\[
\text{Area}(\Omega) = 2 \int_{x_A}^{x_B} \sqrt{-g(x)} dx.
\]

We are going to show that if \( C \) is quantized in the sense above, we can associate to it a solution \( \psi(x) = Re^{iS(x)/\hbar} \) of some stationary Schrödinger equation. Choose a number \( E > 0 \) and define two functions \( S(x) \) and \( V(x) \) by
\[
f(x) = S'(x) \quad , \quad g(x) = 2m(V(x) - E)
\]
that is
\[ S(x) = \int_{x_0}^{x} f(x')dx' \, , \, V(x) = \frac{g(x)}{2m} + E \]  \hspace{1cm} (24)
where \( x_0 \) is an arbitrary fixed number. Eqn. (21) for \( C \) is then
\[ \frac{1}{2m}(p - S'(x))^2 + V(x) - E = 0. \]  \hspace{1cm} (25)
Consider the differential operator
\[ \frac{1}{2m} \left( -i\hbar \frac{d}{dx} - S'(x) \right)^2 + V(x); \]

it has a discrete spectrum consisting of positive eigenvalues. Let \( E_0 \) be the smallest eigenvalue; the boundary of \( \Omega \) must thus satisfy the quantization condition (13), that is
\[ \int_{x}^{x_B} \sqrt{2m|E - V(x)|}dx = \int_{x}^{x_B} \sqrt{2m|E_0 - V(x)|}dx + \frac{Nh}{2}. \]
This condition determines the value \( E \). Let us now look for a function \( R(x) \) such that
\[ V(x) - E = \frac{\hbar^2}{2m} \frac{R''(x)}{R(x)} \]  \hspace{1cm} (26)
that is
\[ -\frac{\hbar^2}{2m}R''(x) + (V(x) - E)R(x) = 0. \]  \hspace{1cm} (27)
The function \( \psi(x) = Re^{iS(x)/\hbar} \) is a solution of the equation
\[ \left[ \frac{1}{2m} \left( -i\hbar \frac{\partial}{\partial x} - S'(x) \right)^2 + V(x) \right] \psi(x) = 0 \]
as is shown by a direct calculation using the identity (27); \( \psi(x) \) is, therefore, the wave-function we are looking for. Notice that the choice of the value \( x_0 \)
in (24) is irrelevant because if we replace it with another value \( x_0' \neq x_0 \) it changes \( \psi \) into \( \psi' = e^{i\gamma/\hbar}\psi \) where \( \gamma = \int_{x_0}^{x_0'} f(x')dx' \) is a constant phase.

5 Examples

5.1 Squeezed states

We consider (unnormalized) squeezed coherent states
\[ \psi_{a,b}(x) = e^{-\frac{1}{2}(a+ib)x^2} \]  \hspace{1cm} (28)
where \(a\) and \(b\) are real and \(a > 0\). The functions \(S(x) = -\frac{1}{2} bx^2\) and \(R(x) = e^{-ax^2/2\hbar}\) satisfy

\[
S'(x) = -bx, \quad \frac{R''(x)}{R(x)} = -\frac{a}{\hbar} + \frac{1}{\hbar^2}a^2 x^2. \tag{29}
\]

The Fermi function of \(\psi_{a,b}\) is thus the quadratic form

\[
g_F(x,p) = (p + bx)^2 + a^2 x^2 - a\hbar. \tag{30}
\]

Setting \(z = (x, p)\) we can rewrite formula (30) as

\[
g_F(x,p) = z^T M z - a\hbar
\]

where \(M\) is the symmetric matrix

\[
M = \begin{pmatrix} a^2 + b^2 & b \\ b & 1 \end{pmatrix}. \tag{31}
\]

Since \(\det M = a^2\) it follows that the surface \(\Omega\) enclosed by the ellipse \(C : g_F(x,p) = 0\) is \(\frac{1}{2} \hbar\).

A straightforward calculation shows that the matrix (31) factorizes as

\[
M = S^T \begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix} S \tag{32}
\]

where \(S\) is the unimodular matrix

\[
S = \begin{pmatrix} a^{1/2} & 0 \\ a^{-1/2} b & a^{-1/2} \end{pmatrix}. \tag{33}
\]

It turns out –and this is really a striking fact!– that \(M_F\) is closely related to the Wigner transform

\[
W\psi_{a,b}(z) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{-\frac{i\hbar}{2} y} \psi_{a,b}(x + \frac{1}{2} y) \psi_{a,b}^*(x - \frac{1}{2} y) dy. \tag{34}
\]

of the state \(\psi_{a,b}\). In fact (see e.g. de Gosson [8], Littlejohn [15]),

\[
W\psi_{a,b}(z) = (\pi\hbar)^{-1/2} a^{-1/2} e^{-z^T G z / \hbar} \tag{35}
\]

where \(G\) is the matrix

\[
G = S^T S = \begin{pmatrix} a + b^2/a & b/a \\ b/a & 1/a \end{pmatrix}. \tag{36}
\]
It follows from Eqn. (32) that
\[ W\psi_{a,b}(z) = (\pi\hbar)^{-1/2}(\det a)^{-1/2}e^{-a}\exp \left[-\frac{1}{\hbar}g_F(S^{-1}D^{-1/2}Sz)\right] \] (37)
with \( D = \begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix} \).

In particular, when \( n = 1 \) and \( \psi_{a,b}(x) = e^{-x^2/2\hbar} \) we have \( S^{-1}D^{-1/2}S = I \) and \( a = 1 \) and hence
\[ W\psi(z) = (\pi\hbar)^{-1/4}e^{-1/\pi^2}e^{-\frac{1}{\pi^2}Mz} \]
which was already noticed by Benenti and Strini [4].

5.2 Hermite functions

The \( N \)-th Hermite function is
\[ h_N(x) = (\sqrt{\pi}2^N N!)^{-1/2}e^{-Q^2/2}H_N(Q), \quad Q = \left(\frac{m\omega}{\hbar}\right)^{1/2}x \] (38)
where
\[ H_N(x) = (-1)^N e^{x^2} \frac{d^N}{dx^N} e^{-x^2} \] (39)
is the \( N \)-th Hermite polynomial; the latter satisfies the second-order differential equation
\[ H_N''(x) - 2xH_N'(x) + 2nH_N(x) = 0. \] (40)
Here, \( S(x) = 0 \) and a straightforward calculation using the relation (40) yields
\[ \frac{R''(x)}{R(x)} = \frac{m^2\omega^2}{\hbar^2}x^2 - (2N + 1)\frac{m\omega}{\hbar}; \] (41)
hence the Fermi function is here
\[ g_F(x,p) = p^2 + m^2\omega^2x^2 - (2N + 1)m\omega\hbar. \] (42)
The curve \( C : g_F(x,p) = 0 \) is again an ellipse, enclosing a surface \( \Omega \) with area
\[ \text{Area}(\Omega) = (N + \frac{1}{2})\hbar. \] (43)

This example is not very instructive, because the Fermi operator \( \hat{g}_F \) is, up to the factor \( 1/2m \) just \( \hat{H} - (N + \frac{1}{2})\hbar\omega \) where
\[ \hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2 \]
is the harmonic oscillator Hamiltonian, whose eigenstates are precisely the
Hermite functions (38). We leave it to the reader to verify that the same sit-
uation occurs for every real function which is an eigenstate of some arbitrary
operator
\[ \hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V. \]

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