COMPLEX GAUSSIANS AND THE PAULI NON-UNIQUENESS

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Received 4 February 1987; accepted for publication 13 April 1987
Communicated by J.P. Vigier

The eigenvalue equations for the complex Pauli unique gaussians as well as for the non-unique ones are given, and the general solutions to them are outlined. In addition, it is proved that not all real states are Pauli unique.

Recently, complex gaussians have been exploited as basis functions for a description of molecular motions which include vibrations in the semiclassical approach [1], for a comparison of quantum and classical mechanics [2], with electronic structure investigations [3], etc. The gaussians were in general given [1] by

$$\psi_k = C\exp[-a_k(q-q_0)^2 + \mathrm{i}p_0(q-q_0)/\hbar] ,$$

$$k=1,2 ,$$

as well as by ψ_k^*, where $\mathrm{Re}(a_k)>0$, $C=[2\,\mathrm{Re}(a_k)/\hbar]^{1/4}$, and $a_2=a_1^*$. The last relation implies $\mathrm{Re}(a_2)=\mathrm{Re}(a_1)$, and $\mathrm{Im}(a_2)=-\mathrm{Im}(a_1)$, and in the following we shall refer to these expressions as $\mathrm{Re}(a)$ and $\pm\mathrm{Im}(a)$, respectively. For the same reason we shall write $|a_2|=|a_1|=|a|$.

Two main features of the gaussians were important for choosing them as basis functions: the localization of the wave packet at $|\langle\hat{q}\rangle|=q_0$ and $|\langle\hat{p}\rangle|=p_0$, and the position–momentum correlation introduced by the $\mathrm{Im}(a)$ term. The former feature can be characterized, and elaborated further, by "bound states in which the particle is restrained by external forces (potential energy) to a particular region in space" [4]. It is therefore of interest to investigate which hamiltonians possess the considered gaussians as their eigenfunctions and whether ψ_1 and ψ_2 (ψ_1^* and ψ_2^*) are uniquely determined by their position and momentum distribution (i.e. whether they are Pauli unique, to which question we answered in the negative in ref. [5]).

It is shown below that ψ_k is the eigenfunction of H_k whose potential part is complex no matter whether $\mathrm{Im}(a)=0$ or not [‡1]. As for the afore-mentioned Pauli non-uniqueness we showed in ref. [5] that $\langle\hat{p}\rangle_{\psi_1}=\langle\hat{p}\rangle_{\psi_2}=p_0$, $\langle\hat{q}\rangle_{\hat{\psi}_1}=\langle\hat{q}\rangle_{\hat{\psi}_2}=q_0$ (where $\hat{\psi}_1$ and $\hat{\psi}_2$ are Fourier transforms of ψ_1 and ψ_2), and, in effect, $\langle\hat{H}_1\rangle_{\psi_1}=\langle\hat{H}_1\rangle_{\psi_2}=\langle\hat{H}_2\rangle_{\psi_1}=\langle\hat{H}_2\rangle_{\psi_2}=E$. On the other hand, the gaussian with $\mathrm{Im}(a)=0$ (in which case $\psi_1=\psi_2$) belongs to the "real states" and is therefore Pauli unique [8]. However, in ref. [8] the question "are all real states Pauli unique?" remained unanswered and we shall eventually fill in this gap.

Let us consider the hamiltonian $\hat{H}_k=\hat{p}^2+\hat{V}_k$, $k=1$, 2, whose domain is $D(H_k)\subset L_2(-\infty,+\infty)$, which is self adjoint, and where $\hat{V}_k$ is the multiplication operator whose representative function is

$$V_k(q)=\hbar a_k[2\hbar a_k(q-q_0)^2-2\mathrm{i}p_0(q-q_0)$$

$$-\mathrm{i}\hbar\,\mathrm{Im}(a_k)/\mathrm{Re}(a)]/m, \quad k=1,2 .$$

The eigenvalue equation is given by

[‡1] The hamiltonian to which ref. [5] should be considered to refer is $\hat{H}_k$. Its potential part is complex, and given by $\hat{V}_k$ defined in the following, and not real as put in ref. [5]. I gratefully acknowledge S. Epstein [6], who drew my attention to the fact that a hamiltonian with a real potential part cannot have ψ_k as its eigenfunction. As to the complex potential it was used in quantum mechanics as early as 1954 [7].

$$\hat{H}_k\phi_k = (\hat{p}^2 + \hat{V}_k)\phi_k = -(\hbar^2/2m)\phi_k'' + V_k(q)\phi_k = E\phi_k,$$

$$k=1,2, \qquad (1)$$

where $\phi_k'' = d^2\phi_k/dq^2$. (We shall use the notation $f' = df/dq$, and $f'' = d^2f/dq^2$ throughout.)

ψ_k obviously satisfies eq. (1) for $E = p_0^2/2m + \hbar^2|a|^2/m\,\mathrm{Re}(a)$. In order to get a general solution to eq. (1) let us introduce the polynomial

$$P_k = \sum_{j=0}^{\infty} c_{(j)k}[2a_k(q-q_0) - \mathrm{i}p_0/\hbar]^j, \quad k=1,2,$$

and substitute $\phi_k = P_k\psi_k$ into eq. (1). We obtain the following equation:

$$P_k'' - 4a_k(q-q_0)P_k' + rP_k = 0, \quad k=1,2, \qquad (2)$$

where $r = 2mE/\hbar^2 - p_0^2/\hbar^2 - 2|a|^2/\mathrm{Re}(a)$. In order for this equation to be valid for any q the coefficient of each q^j must be zero. On the other hand, since eq. (1) has one irregular singularity at infinity [9], P_k must terminate for ϕ_k to be from $L_2(-\infty, +\infty)$. Let it terminate at $j=n$. Then the recursion relation obtained for the highest potention of q, i.e. q^n,

$$(n+1)(n+2)c_{(k)n+2} + (r - 4a_k n)c_{(k)n} = 0,$$

$$k=1,2, \qquad (3)$$

implies $r = 4a_k n$, and therefore P_k is wholly even or odd according to n being even or odd.

Therefore, in case $\mathrm{Im}(a_k)=0$ we finally have

$$E_n = p_0^2/2m + \hbar^2\,\mathrm{Re}(a)(2n+1)/m,$$

and

$$\phi_1 = \phi_2 = \sum_{j=0}^{n} c_j[2\,\mathrm{Re}(a)(q-q_0) - \mathrm{i}p_0/\hbar]^j$$

$$\times \exp[-\mathrm{Re}(a)(q-q_0)^2 + \mathrm{i}p_0(q-q_0)/\hbar],$$

where $c_{n-1} = c_{n-3} = \ldots = 0$, and the other c_j are given by (3).

In case $\mathrm{Im}(a_k) \neq 0$, n has to be zero in order for E to be real and consequently $\phi_k = \psi_k$. This does not mean that ψ_k is the only possible solution to eq. (1); however, the second solution which is of the following form [9]:

$$c\psi_k \int \exp(-Aq^3 + Bq^2 + Dq)\,dq, \quad \mathrm{Re}(A) > 0,$$

as well as the linear combination of the two do not belong to $L_2(-\infty, +\infty)$, since eq. (1) has one singular point at infinity. And, as shown above, the appropriate sequences cannot be terminated in the usual way (i.e. the one which would directly determine the particular discrete energies). Of course, approximations which belong to $L_2(-\infty, +\infty)$ are always possible (e.g. by means of hypergeometric functions), but it seems they have to be adapted to the particular problem in question, and we shall not consider the case any further. However, we would like to draw the reader's attention to an ambiguity which emerges from the obtained results. The complex gaussians with $\mathrm{Im}(a) \neq 0$ have been introduced in order to describe the position–momentum correlation, which is by itself considered as a missing element in our state description [10], and, on the other hand, it has been shown in ref. [5] that the considered gaussians, though not experimentally indistinguishable, cannot be distinguished with the help of the commonly used observables. Thus it seems worth searching for such new observables which would distinguish between the states.

What we are left with is to answer the question "are all real states Pauli unique?" [8].

For the reader's convenience we shall briefly restate the problem, and give the relevant definitions.

A state is considered to be real if at least one of its representative functions $\psi(q)$ (and/or one of its Fourier transforms) is real. (The afore-defined ψ_k with $\mathrm{Im}(a)=0$ is an example of the real state.) In the following we assume, without a loss in generality, $\psi(q)$ be real. We also assume $\psi(q)$ be square integrable, i.e. belong to $L_2(-\infty, +\infty)$.

A function $(\tilde{\psi}(q))$ is considered a proper Pauli non-unique "partner" of (real) $\psi(q)$ if $\tilde{\psi}(q) = \psi(q)\exp[-\mathrm{i}\vartheta(q)]$, where $\vartheta(q) \neq \mathrm{const}$. (For in this case ψ and $\tilde{\psi}$ are linearly independent [5].) The Pauli non-unique partners have the same position and momentum distribution [5], but not necessarily the same energy. As an example of such Pauli non-unique bound states can serve the ones of the harmonic oscillator [4]. The Pauli non-unique partners with the same energy are, however, much more interesting and we shall concentrate on them.

Let us consider a general real state where ψ and $\tilde{\psi}$ are from the domain of the same self-adjoint hamiltonian $\hat{H}$, whose domain is $D(\hat{H}) \subseteq D(\hat{H}) \subseteq L_2(-\infty, +\infty)$, and let it be

$$\langle \hat{H} \rangle_{\bar{\psi}} = \langle \hat{H} \rangle_{\psi} \,. \tag{4}$$

It is proved in ref. [8] that such a real state can be nothing but Pauli unique, however, subjected to the additional condition that the mean values from (4) are bounded. Briefly, it boils down to the consideration of eq. (4) which reads

$$\langle (\hbar\vartheta')^2/2m - i\hbar^2(\vartheta'' + 2\vartheta'\hat{p})/2m + \hat{H} \rangle_{\psi}$$
$$= \langle \hat{H} \rangle_{\psi} \,. \tag{5}$$

Since $|\langle \hat{H} \rangle_{\psi}| < \infty$ and since $\langle \vartheta'' + 2\vartheta'\hat{p} \rangle_{\psi}$ must be zero for $\langle \hat{H} \rangle_{\psi}$ to be real, it follows that $\langle \vartheta'^2 \rangle_{\psi} = 0$, which is equivalent to $\vartheta'^2 = 0$. Hence $\vartheta = \text{const.}$ Obviously, the obtained result must hold whenever ψ is an eigenfunction of $\hat{H}$ belonging to a finite eigenvalue, since then $\hat{H}\psi$ is from $L_2(-\infty, +\infty)$, and the boundness of (4) follows from the Schwarz inequality.

Let us now lift the assumption that the mean values from (4) are bounded and choose $\psi = |q|^{-3/2}\sin^2 q$, and $\vartheta = \cos q$. There exists the following improper absolutely convergent Riemann integral:

$$\int_{-\infty}^{\infty} \psi^2 \, dq = \lim_{\substack{\epsilon,\eta \to 0 \\ \lambda,\nu \to \infty}} \left(\int_{-\lambda}^{-\epsilon} \psi^2 \, dq + \int_{\eta}^{\nu} \psi^2 \, dq \right) = \ln 4$$

and since $\psi^2 = \bar{\psi}^* \bar{\psi}$ itself is (Lebesgue) measurable, the Riemann integral coincides with the Lebesgue one. Hence ψ belongs to $L_2(-\infty, +\infty)$, as well as $\bar{\psi}$. All the other integrals we are going to consider will too be either absolutely covergent or not (and therefore intinite in the sense of Lebesgue).

In order for ψ and $\bar{\psi}$ to give the same momentum distribution the following equation has to be satisfied,

$$-i \int_{-\infty}^{\infty} \psi^2 \vartheta' \, dq + \int_{-\infty}^{\infty} \psi\psi' \, dq = \int_{-\infty}^{\infty} \psi\psi' \, dq$$

and this is, given our functions, accomplished since both integrals are absolutely convergent and equal to zero. The equality of the position distributions follows directly from: $\bar{\psi}^* \bar{\psi} = \psi^* \psi = \psi^2$.

The middle term from (5) boils down to (the integral on the left side exists, i.e. converges absolutely):

$$\int_{-\infty}^{\infty} (\psi^2 \vartheta'' + 2\psi\psi'\vartheta') \, dq = \int_{-\infty}^{\infty} (\psi^2 \vartheta')' \, dq$$
$$= \psi^2 \vartheta' \Big|_{-\infty}^{\infty} = 0$$

and the desired reality of (5) is achieved. Since, as can be easily checked, $\int_{-\infty}^{\infty} \psi\psi'' dq = \infty$ (hence, according to the Schwarz inequality, $\psi'' \notin L_2(-\infty, +\infty)$) in the sense of Lebesgue, as well as of Riemann, we need not have (for a suitable choice of $V(q)$) $\langle \vartheta'^2 \rangle_{\psi} = 0$ in order to satisfy eq. (5). (In fact, we can show that $\langle \vartheta'^2 \rangle_{\psi} = 3(8 \ln 2 - 3 \ln 3)/8$.)

Thus we have answered the considered question in the negative, contrary to the conjecture expressed in ref. [8].

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