Minimum uncertainty products via the variational principle

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The problem of finding the class of wave packets ψ that minimizes the quantum-mechanical uncertainty product $\Delta_x \Delta_p$ is treated via the constrained variational principle. This leads to a harmonic-oscillator-type wave equation for ψ whose explicit solutions are obtained when the potential V has, or does not have, an infinite step. The method can be fruitfully applied to the quantum cosmology of the inflationary universe.

I. INTRODUCTION

One of the most celebrated problems of wave mechanics in one dimension is to find the optimal normalized wave packet $\psi(x,t)$ that makes the quantum uncertainty product

$$J=\Delta_x^2\Delta_p^2 \tag{1}$$

attain its minimum value. Here Δ_x and Δ_p are the spreads in the position variable x and momentum variable p, respectively, both calculated at *specific* instant of time t. As rigorously demonstrated in textbooks[1-3] through the use of the Schwartz inequality, the least possible value of J is simply $(\hbar/2)^2$, which corresponds to an essentially unique Gaussian-like solution (labeled by the subscript G),

$$\psi_G=\frac{1}{(2\pi\Delta_x^2)^{1/4}}\exp\left[-\frac{(x-\langle x\rangle)^2}{4\Delta_x^2}+\frac{i\langle p\rangle x}{\hbar}\right] . \tag{2}$$

The solution (2) depends on the mean values of $\langle x\rangle$ and $\langle p\rangle$ but is supposedly independent of the form of the underlying potential $V(x)$. The aim of the present paper is to prove the following two new, additional results in the above context.

(i) The question of minimizing the functional J with respect to ψ can be viewed as a problem of *variational calculus.* As demonstrated in Sec. II, this leads to a set of variational conditions on the wave function ψ as well as on some Lagrange multipliers λ.

(ii) The solution of the said conditions, in general, leads to an infinite set of wave functions ψ [called the generalized minimum uncertainty packets (GMUP)], each of which corresponds to a local minimum of J. The explicit forms of GMUP are determined in Sec. III for two cases, viz., when the range of x is unrestricted from $-\infty$ to ∞ because V has no infinite step, and when x is restricted from 0 to ∞ (say) because V has an infinite step. In the former case the conventional solution ψ_G of (2) is *allowed,* but in the latter case it is *ruled out.*

II. VARIATIONAL FORMALISM

We wish to minimize the uncertainty product [cf. Eq. (1)] subject to the constraints that the state should have the correct normalization, position mean, and momentum mean equal to 1, $\langle x\rangle$, and $\langle p\rangle$, respectively. For this purpose we define the quantities

$$\begin{aligned}R_j&=\int dx\,\psi^* x^j\psi,\quad j=0,1,2\\ S_j&=\int dx\,\psi^* p^j\psi,\quad p=-i\hbar\frac{\partial}{\partial x}\end{aligned} \tag{3}$$

which are assumed to be finite with the limits of x integration depending upon the physical problem. The dispersions in the x and p variables are given by

$$\begin{aligned}\Delta_x^2&=R_2/R_0-(R_1/R_0)^2 ,\\ \Delta_p^2&=S_2/S_0-(S_1/S_0)^2 .\end{aligned} \tag{4}$$

Note the functional derivatives

$$\delta R_j/\delta\psi^*=x^j\psi,\quad \delta S_j/\delta\psi^*=p^j\psi . \tag{5}$$

The objective function to be minimized is

$$\begin{aligned}\bar J=&\Delta_x^2\Delta_p^2+2\bar\lambda_1(R_1/R_0-\langle x\rangle)\\ &+2\bar\lambda_2(S_1/S_0-\langle p\rangle)+2\bar\lambda_3(R_0-1) ,\end{aligned} \tag{6}$$

where the $\bar\lambda$'s are Lagrange multipliers. When we set the partial derivatives

$$\partial\bar J/\partial\bar\lambda_3=\partial\bar J/\partial\bar\lambda_1=\partial\bar J/\partial\bar\lambda_2=0 ,$$

we retrieve the constraint equations

$$R_0=1,\quad R_1=\langle x\rangle,\quad S_1=\langle p\rangle . \tag{7}$$

The imposition of $\delta\bar J/\delta\psi^*=0$ is readily effected using Eqs. (5) and (6) and yields a differential equation for the optimum ψ as

$$[\Delta_x^2(p-\langle p\rangle+\lambda_2)^2+\Delta_p^2(x-\langle x\rangle+\lambda_1)^2-E]\psi=0 , \tag{8a}$$

with

$$\begin{aligned}&\lambda_1=\bar\lambda_1/\Delta_p^2,\quad \lambda_2=\bar\lambda_2/\Delta_x^2,\quad \bar\lambda_3=0 ,\\ &E=\Delta_x^2\lambda_2^2+\Delta_p^2\lambda_1^2+2\Delta_x^2\Delta_p^2 .\end{aligned} \tag{8b}$$

Next, writing in Eq. (8a),

$$X=x-\langle x\rangle+\lambda_1\ ,$$
$$\psi=f\exp[i(\langle p\rangle-\lambda_2)X/\hbar]\ , \tag{9a}$$

the wave equation for f emerges in the form of a linear harmonic oscillator,[4] viz.,

$$-\Delta_x^2\hbar^2\frac{\partial^2 f}{\partial X^2}+\Delta_p^2X^2f=Ef\ . \tag{9b}$$

The parameters λ_1 and λ_2 [cf. Eq. (8b)] are fixed imposing constraints (7) as

$$\lambda_1=\int dX\,f^*Xf\ ,$$
$$\lambda_2=-i\hbar\int dX\,f^*\frac{\partial f}{\partial X}\ , \tag{10}$$

where the range of X depends on the physical problem. The question of solving Eq. (9b) subject to the constraints (10) will be taken up in the next section.

III. SOLUTIONS

A. General considerations

Following the treatments of Schiff[4] and of Morse and Feshbach,[5] a pair of standard, linearly independent solutions of Eq. (9b) can be denoted by u_n, v_n belonging to the eigenvalue E such that

$$u_n=H_n(\alpha X)\exp(-\tfrac{1}{2}\alpha^2X^2)\ ,$$
$$v_n=u_n\int^X dX'\frac{1}{u_n^2(X')},\quad \alpha=\left[\frac{\Delta_p}{\hbar\Delta_x}\right]^{1/2}\ , \tag{11}$$
$$E=(n+\tfrac{1}{2})\hbar w,\quad w=2\Delta_x\Delta_p\ ,$$

with H_n being the Hermite polynomials of order $n=0,1,2,\ldots$. In general, f will be a linear combination of u_n, v_n; also, a relation between Δ_p and Δ_x will emerge upon equating the two formulas [(8b), (11)] of E. To be more precise, let us take the following cases in Secs. III B and III C.

B. V has no infinite steps

Here the allowed range of x is $(-\infty,\infty)$. Due to the normalization requirement only the u_n type of solution is permitted so that $f\propto u_n$. By parity arguments both the integrals appearing on the right-hand side of Eq. (10) vanish yielding $\lambda_1=\lambda_2=0$. Comparison of the two formulas [(8b) and (11)] of E gives

$$\Delta_x\Delta_p=(n+\tfrac{1}{2})\hbar,\quad \alpha=[(n+\tfrac{1}{2})/\Delta_x^2]^{1/2}\ . \tag{12}$$

The normalized expression of GMUP becomes [cf. Eq. (9a)]

$$\psi=N_n\exp(i\langle p\rangle X/\hbar)u_n\ , \tag{13}$$

where $N_n=(\alpha/\pi^{1/2}2^nn!)^{1/2}$ and $X=x-\langle x\rangle$. Note that our ψ and the conventional ψ_G [cf. Eq. (2)] coincide to within a constant phase factor for $n=0$.

At this juncture it is worth mentioning that the existence of the sequence (12) of uncertainty products has been known in the literature in a totally *different* context, viz., construction of coherent-state solutions for the harmonic oscillator[6] and for generalized potentials.[7] These authors have not attempted the minimization of $\Delta_x\Delta_p$ through the variational principle for unknown V.

C. V has one infinite step

If $V(x)=-\infty$ for $-\infty<x<0$, then the allowed range of x is $(0,\infty)$ and every physical wave function must satisfy

$$\psi(0,t)=0\ . \tag{14}$$

Again, normalizability demands that only u_n-type solutions be picked up for f. The choice $f\propto u_0$, i.e., $\psi\propto\psi_G$ is ruled out because ψ_G cannot vanish at any finite x. We shall, however, show that $f\propto u_1$ is perfectly valid in the sense that all quantum-mechanical requirements are fulfilled. Indeed, u_1 vanishes at $x=0$ if $\lambda_1=\langle x\rangle$. Now $X=x$ so that the normalization condition $\langle f\,|\,f\rangle=1$ leads to $f=(\alpha/\sqrt{\pi})^{1/2}u_1$. From Eq. (10) we can easily compute $\lambda_1=2/\alpha\sqrt{\pi}$ and $\lambda_2=0$. By inserting these values of λ into Eq. (8b) and comparing with Eq. (11) for E (with $n=1$), we get

$$\Delta_x\Delta_p=(\tfrac{3}{2}-2/\pi)\hbar\approx 0.87\hbar\ ,$$
$$\psi=\left[\frac{\alpha}{\sqrt{\pi}}\right]^{1/2}\exp\left[\frac{i\langle p\rangle X}{\hbar}\right]u_1\ , \tag{15}$$

with $\alpha\approx(0.87/\Delta_x^2)^{1/2}$ and $X=x$ here.

IV. DISCUSSION

With regard to the formalism developed in Sec. II and the solutions obtained in Sec. III, the following comments are in order.

(1) Note that the solutions (13) and (15) contain parameters $\langle x\rangle,\langle p\rangle,\Delta_x^2,\Delta_p^2$, which depend on the knowledge of ψ itself in view of definitions (3) and (4). In order to demonstrate the existence of these solutions we must check for self-consistency. This is readily done by recalling the definition of u_n [see Eq. (11)] along with the properties of Hermite polynomials. For example, in the case of solution (13) the consistency check for the average value of position goes as

$$\langle x\rangle=\int_{-\infty}^{\infty}dx\,\psi^*x\psi$$
$$=\int_{-\infty}^{\infty}dX(X+\langle x\rangle)N_n^2u_n^2=\langle x\rangle\ . \tag{16}$$

Similarly, one can explicitly verify for $\langle p\rangle$, etc.

(2) Notice that the sequence of GMUP solutions obtained in Eq. (11) are characterized by $n=0,1,2,3,\ldots$ nodes, respectively. The solution with $n=0$ is well known in textbooks; it corresponds to the *least* possible value of $\Delta_x\Delta_p$, viz., $\hbar/2$. The solutions with $n\geq 1$ are new; these correspond to the remaining possible *extrema* (i.e., local minima and maxima) of $\Delta_x\Delta_p$ regarded as a functional of ψ. These extra solutions with $n\geq 1$ are needed when the potential V has one, two or more infinite steps.

Therefore, our method of generating GMUP works successfully for different shapes of the physical potential. This should be very useful in practical applications because such a GMUP may be regarded to supply the *initial* condition at $t=0$, say, in a wave-mechanical problem. This statement is particularly relevant in the context of quantum cosmological models applied to the inflationary universe when infinite step potentials are used.

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