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THE TIME DEPENDENT VARIATIONAL PRINCIPLE DESCRIPTION OF THE MOTION OF A GAUSSIAN WAVE PACKET

by

C.P. Malta and M.A. Martinez de Aguiar
Instituto de Física, Universidade de São Paulo

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C.P. Malta and M.A. Martinez de Aguiar†

Universidade de São Paulo, Instituto de Física, Depto. de Física Matemática, CP 20516, 01498 São Paulo, SP, Brazil

ABSTRACT

As an illustration, the time dependent variational principle with parametrized wave function is applied to describe the free motion of a gaussian wave packet and its deformation when interacting with a potential barrier.

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I. INTRODUCTION

The time dependent variational principle (TDVP) (introduced by Dirac[1] in 1930) has proved to be a useful tool in generating approximate solutions in nuclear physics problems. Different types of approximate solutions are obtained by using the variational principle restricted to a subspace of the Hilbert space. The time dependent Hartree-Fock theory[2,3], for instance, is the result of using the variational principle in the subspace of Slater determinants.

The most convenient way of using the TDVP is by parametrizing the trial wave function. The parametrized wave function will span a subspace of the Hilbert space and using it in the TDVP obtains classical equations of motion for the chosen parameters[4,5]. A particular subspace of the Hilbert space is selected by appropriately choosing the parameters, guided by the physical collective aspect of the system to be investigated.

The interesting feature of this method is that it provides some quantum information despite the classical character of the parameters equations of motion. Of course there are also quantum informations that cannot be directly extracted from those classical equations and require previously some requantization procedure such as WKB or Bohr-Sommerfeld[6].

The main purpose of this work is to apply the method of parametrized TDVP in describing the motion of a gaussian wave packet when interacting with a potential barrier. It is a simple example but of great pedagogical value as it completely illustrates the method, including the procedure for choosing the parametrization. In section II we derive the equations for a parametrized trial function and in section III apply it to describe the deformation of a gaussian wave packet due to its interaction with a potential barrier. In section IV we describe the free motion (no barrier) of the wave packet and, for small time intervals, its spreading is shown to be exactly as predicted by quantum mechanics. In section V we present the results for the case of an exponential barrier and the conclusions are summarized in section VI.

II. THE TDVP AND THE CLASSICAL EQUATIONS OF MOTION

The TDVP may be described as a principle of least action[4,5]. The action is given by

$$S = \int_{t_1}^{t_2} L(\psi,\bar{\psi})\,dt \quad , \tag{2.1}$$

with the real Lagrangian

$$L(\psi,\bar{\psi}) = \frac{i\hbar}{2}\,\frac{\langle\psi|\dot{\psi}\rangle - \langle\dot{\psi}|\psi\rangle}{\langle\psi|\psi\rangle} - \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \quad , \tag{2.2}$$

where H is the Hamiltonian of the system and $|\psi\rangle$ a unnormalized wave function (the bar indicates complex conjugation and the dot time derivative). And the TDVP is given by

$$\delta S = 0 \quad , \tag{2.3}$$

with the boundary conditions

$$\delta|\psi(t_1)\rangle = \delta|\psi(t_2)\rangle = \delta\langle\psi(t_1)| = \delta\langle\psi(t_2)| = 0 \quad . \tag{2.4}$$

It is easy to see that unconstrained variations of $|\psi\rangle$ and $\langle\psi|$ lead to the time dependent Schrödinger equation (TDSE) for unnormalized wave-function

$$(i\hbar\frac{\partial}{\partial t} - H)|\psi\rangle = \frac{\langle\psi|\frac{i\hbar}{2}\frac{\partial}{\partial t} - H|\psi\rangle}{\langle\psi|\psi\rangle}\,|\psi\rangle \quad , \tag{2.5}$$

and its adjoint equation.

The nice feature of this method is that approximations are naturally obtained by restricting the variations of $\langle\psi|$ and $|\psi\rangle$ to a subspace of the Hilbert space. A simple way of doing this is by parametrizing the trial function $|\psi\rangle$. Depending on the parameter choice, a particular subspace of the Hilbert space will be selected. We shall consider the wave function parametrized in terms of a set of complex parameters $\underset{\sim}{z} = (z_1, z_2, \ldots, z_r)$, and we shall write

$$|\psi(t)\rangle = |\underset{\sim}{z}(t)\rangle \quad . \tag{2.7}$$

Of course, the particular choice of parameters depends on the problem to be solved as they are related to some collective modes of the physical system. We shall consider two cases of parametrization that will be useful for our purposes:

(i) $|\underset{\sim}{z}(t)\rangle$ depends only on $\bar{\underset{\sim}{z}}$;

(ii) $|\underset{\sim}{z}(t)\rangle$ depends on both $\underset{\sim}{z}$ and $\bar{\underset{\sim}{z}}$.

Case (i) has been treated in many other papers[5,6,7] so we shall make a brief review only. The Lagrangian in this case reads

$$L(z,\bar{z}) = \frac{i\hbar}{2}\sum_{i=1}^{r}\left[\dot{\bar{z}}_i\,\frac{\partial}{\partial\bar{z}_i} - \dot{z}_i\,\frac{\partial}{\partial z_i}\right]\ell n\,N - H \quad , \tag{2.8}$$

where

$$N(\underset{\sim}{z},\bar{\underset{\sim}{z}}) = \langle \underset{\sim}{z} | \underset{\sim}{z} \rangle \tag{2.9}$$

and

$$H(\underset{\sim}{z},\bar{\underset{\sim}{z}}) = \frac{\langle \underset{\sim}{z} | H | \underset{\sim}{z} \rangle}{N} \quad . \tag{2.10}$$

Variations of the action (2.1) with respect to z_i and $\bar{z}_i$ leads to the system of equations

$$i\hbar\, \dot{\bar{z}}_i = \sum_j (g^{-1})_{ij} \frac{\partial H(\underset{\sim}{z},\bar{\underset{\sim}{z}})}{\partial z_j} \quad \text{and} \quad \text{c.c.} \quad , \tag{2.11}$$

where the matrix

$$g_{ij} = \frac{\partial^2 \ell n\, N(\underset{\sim}{z},\bar{\underset{\sim}{z}})}{\partial z_i\, \partial \bar{z}_j} \tag{2.12}$$

is assumed to be invertible ($\det g \neq 0$).

Defining a generalized Poisson brackets of functions of z and $\bar{z}$ as

$$\{F,G\} = \sum_{ij} \left\{ \frac{\partial F}{\partial \bar{z}_i} (g^{-1})_{ij} \frac{\partial G}{\partial z_j} - \frac{\partial G}{\partial \bar{z}_i} (g^{-1})_{ij} \frac{\partial F}{\partial z_j} \right\} \quad , \tag{2.13}$$

equations (2.11) assume an explicit canonical form:

$$i\hbar\, \dot{\bar{z}}_k = \{z_k, H\} \quad . \tag{2.14}$$

Case (ii) is a bit more complicated. In that case the Lagrangian (2.2) reads

$$L(\underset{\sim}{z},\bar{\underset{\sim}{z}}) = \sum_{i=1}^{r} \dot{z}_i\, \chi_i + \dot{\bar{z}}_i\, \bar{\chi}_i - H \quad , \tag{2.15}$$

where we have defined

$$\chi_i = \frac{i\hbar}{2} \, \frac{\langle \underset{\sim}{z} | \frac{\overrightarrow{\partial}}{\partial z_i} | \underset{\sim}{z} \rangle - \langle \underset{\sim}{z} | \frac{\overleftarrow{\partial}}{\partial z_i} | \underset{\sim}{z} \rangle}{N} \quad ,$$

the arrows indicating the side on which the operator is acting. The stationarity of the action with respect to $\underset{\sim}{z}_i$ and $\bar{\underset{\sim}{z}}_i$ leads to the following system of equations:

$$\dot{z}_j \left(\frac{\partial \chi_j}{\partial z_i} - \frac{\partial \chi_i}{\partial z_j} \right) + \dot{\bar{z}}_j \left(\frac{\partial \bar{\chi}_j}{\partial z_i} - \frac{\partial \chi_i}{\partial \bar{z}_j} \right) = \frac{\partial H}{\partial z_i} \quad . \tag{2.16}$$

As we can see, these equations are far from the desirable canonical form. However, in the particular case of one parameter these equations are very simple because the first term on the left goes to zero and we get

$$\begin{aligned} \dot{\bar{z}} &= \left(\frac{\partial \bar{\chi}}{\partial t} - \frac{\partial \chi}{\partial \bar{z}} \right)^{-1} \frac{\partial H}{\partial z} \quad , \\ \dot{z} &= \left(\frac{\partial \chi}{\partial \bar{z}} - \frac{\partial \bar{\chi}}{\partial z} \right)^{-1} \frac{\partial H}{\partial \bar{z}} \quad . \end{aligned} \tag{2.17}$$

III. THE TRIAL WAVE FUNCTION FOR THE CALCULATION OF DEFORMATION AMPLITUDES

The wave function that will be used for describing the deformation of a wave packet when interacting with a potential barrier will be a combination of parametrizations (i) and (ii) presented in section II.

In many applications of the TDVP the coherent state wave packet has proved to be a useful variational function. It is suitable for describing the elastic scattering of light nuclei[5]. The parameters in this case describe the relative motion of the colliding nuclei and no internal excitation can be described by using this simple parametrization. The undeformable (and unnormalized) coherent state describing the relative motion is written as

$$|z\rangle = e^{\bar{z}\hat{a}^{\dagger}}|0\rangle \tag{3.1}$$

where

$$z = \frac{1}{\sqrt{2}}\left(\frac{q}{b} - i\,b\frac{p}{\hbar}\right) , \tag{3.2a}$$

$$b = \sqrt{\frac{\hbar}{m\omega}} , \tag{3.2b}$$

q and p being the coordinate and momentum parameters respectively, and $|0\rangle$ the ground-state of the harmonic oscillator of energy spacing $\hbar\omega$, $\hat{a}|0\rangle = 0$ (m is the reduced mass of the colliding nuclei).

In our case, as we want to describe the deformation of a wave packet during its interaction with a potential barrier, the natural choice of trial wave function is a superposition of generalized coherent states[8]

$$\begin{aligned} |\underline{z}\rangle &= \sum_{\ell=0}^{\infty} \bar{\alpha}_{\ell}(t)\, e^{\bar{z}\hat{a}^{\dagger}}\, e^{-z\hat{a}}|\ell\rangle \\ &= \hat{W}(z,\bar{z})\,|\underline{\alpha}\rangle , \end{aligned} \tag{3.3}$$

where

$$\hat{W}(z,\bar{z}) = e^{\bar{z}\hat{a}^{\dagger}}\, e^{-z\hat{a}} \tag{3.4}$$

is the unnormalized Weyl operator and

$$|\underline{\alpha}\rangle = \sum_{\ell=0}^{\infty} \bar{\alpha}_{\ell}(t)\,|\ell\rangle \tag{3.5}$$

is a superposition of harmonic oscillator states $|\ell\rangle$ with time dependent amplitudes $\alpha_{\ell}(t)$.

For this parametrized function the norm is given by

$$N(z,\bar{z},\underline{\alpha},\bar{\underline{\alpha}}) = M(z,\bar{z})\,\theta(\underline{\alpha},\bar{\underline{\alpha}}) , \tag{3.6}$$

with

$$M(z,\bar{z}) = e^{z\bar{z}} \quad \text{and} \quad \theta(\underline{\alpha},\bar{\underline{\alpha}}) = \sum_{\ell} |\alpha_{\ell}|^{2}$$

and the Lagrangian (2.2) can be written in the mixed form (compare with (2.8) and (2.15)):

$$L = \frac{i\hbar}{2}\left[\dot{\bar{\underline{\alpha}}}\frac{\partial}{\partial\bar{\underline{\alpha}}} - \dot{\underline{\alpha}}\frac{\partial}{\partial\underline{\alpha}}\right]\ell n\ \theta + \dot{z}\chi + \dot{\bar{z}}\bar{\chi} - H . \tag{3.7}$$

Or,

$$L = A(\underline{\alpha},\bar{\underline{\alpha}}) + \Xi(\underline{\alpha},\bar{\underline{\alpha}},z,\bar{z}) - H(\underline{\alpha},\bar{\underline{\alpha}},z,\bar{z}) \tag{3.8}$$

where

$$\Xi = \dot{z}\chi + \dot{\bar{z}}\bar{\chi} , \tag{3.9}$$

$$H = \frac{\langle\underline{z}|H|\underline{z}\rangle}{N} , \tag{3.10}$$

and

$$\chi = \frac{i\hbar}{2} \frac{\langle \underset{\sim}{z}|\frac{\overrightarrow{\partial}}{\partial z}|\underset{\sim}{z}\rangle - \langle \underset{\sim}{z}|\frac{\overleftarrow{\partial}}{\partial z}|\underset{\sim}{z}\rangle}{N} \tag{3.11a}$$

$$= -\frac{i\hbar}{2}\,\bar{z} - i\hbar \frac{\sum_k \alpha_k\, \bar{\alpha}_{k+1} \sqrt{k+1}}{\sum_k |\alpha_k|^2} \quad . \tag{3.11b}$$

The equations of motion for z, $\bar{z}$, α_i and $\bar{\alpha}_i$ are then obtained by imposing the stationarity of $S = \int L\,dt$, the result being

$$\frac{\partial H}{\partial z} = \dot{\bar{z}} \left(\frac{\partial \bar{\chi}}{\partial z} - \frac{\partial \chi}{\partial \bar{z}}\right) = i\hbar\,\dot{\bar{z}} \quad , \tag{3.12}$$

and its complex conjugate, and

$$\frac{\partial H}{\partial \alpha_k} = i\hbar \sum_j g_{kj}\, \dot{\bar{\alpha}}_j + \dot{z}\, \frac{\partial \chi}{\partial \alpha_k} + \dot{\bar{z}}\, \frac{\partial \bar{\chi}}{\partial \alpha_k} \quad , \tag{3.13}$$

and its complex conjugate, with

$$g_{kj} = \frac{\partial^2\, \ell n\, \theta(\underset{\sim}{\alpha}, \bar{\underset{\sim}{\alpha}})}{\partial \alpha_k\, \partial \bar{\alpha}_j} \quad . \tag{3.14}$$

Equation (3.12) and its complex conjugate describe the translational motion of the wave packet while equation (3.13) describes its deformation.

Now, the equations of motion will have a much simpler form if the parameters can be chosen so as to make the matrix g (3.14) diagonal. In the present case this is achieved by using the normalized amplitudes

$$\beta_\ell = \frac{\alpha_\ell}{\sqrt{\sum_i |\alpha_i|^2}} \quad . \tag{3.15}$$

For this normalized amplitude, the Lagrangian has the form

$$L = \frac{i\hbar}{2} (\dot{\bar{\underset{\sim}{\beta}}}\cdot\underset{\sim}{\beta} - \dot{\underset{\sim}{\beta}}\cdot\bar{\underset{\sim}{\beta}}) + \dot{z}\, \chi(z,\bar{z},\underset{\sim}{\beta},\bar{\underset{\sim}{\beta}}) + \dot{\bar{z}}\, \bar{\chi}(z,\bar{z},\underset{\sim}{\beta},\bar{\underset{\sim}{\beta}}) - H(z,\bar{z},\underset{\sim}{\beta},\bar{\underset{\sim}{\beta}}) \quad , \tag{3.16}$$

with

$$\chi(z,\bar{z},\underset{\sim}{\beta},\bar{\underset{\sim}{\beta}}) = -\, i h \sum_j \sqrt{j+1}\; \beta_j\, \bar{\beta}_{j+1} - \frac{i\hbar}{2}\,\bar{z} \tag{3.17}$$

and the equations of motion are simply

$$i\hbar\, \dot{\bar{\beta}}_j = \frac{\partial H}{\partial \beta_j} - \dot{z}\, \frac{\partial \chi}{\partial \beta_j} - \dot{\bar{z}}\, \frac{\partial \bar{\chi}}{\partial \beta_j}$$

$$= \frac{\partial H}{\partial \beta_j} + \frac{1}{i\hbar} \left\{\frac{\partial H}{\partial \bar{z}}\, \frac{\partial \chi}{\partial \beta_j} - \frac{\partial H}{\partial t}\, \frac{\partial \chi}{\partial \beta_j}\right\} \quad . \tag{3.18}$$

In fact, if we define the effective hamiltonian,

$$h = H + \frac{\hbar^2}{2mb^2} \sum_n (z-\bar{z})\, \sqrt{n+1}\, (\bar{\beta}_n\, \beta_{n+1} - \beta_n\, \bar{\beta}_{n+1}) \tag{3.19}$$

the equations of motion will have the canonical form

$$i\hbar\, \dot{\bar{\beta}}_j = \frac{\partial h}{\partial \beta_j} \quad . \tag{3.20}$$

So, given the Hamiltonian of the system,

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q}) \quad , \tag{3.21}$$

the "deformation amplitudes" $\beta_\ell(t)$ are obtained by solving equations (3.20) (or (3.18)) and (3.12). And the position probability, given by

$$Q(q,t) = \frac{|\langle q|\psi(t)\rangle|^2}{\langle\psi|\psi\rangle} = \sum_\ell |\overline{\beta}_\ell|^2 |\langle q|\ell\rangle|^2 \quad , \tag{3.22}$$

will describe the shape of the packet as function of time.

In order to solve the equations of motion it is necessary to calculate $H(z,\overline{z},\beta,\overline{\beta})$. This is a lengthy calculation done in the Appendix.

In the next section we discuss the free motion $(V(\hat{q}) = 0)$ of the packet for small t and in the following section we calculate the case $V(q) = V_0\, e^{\gamma q}$.

IV. FREE MOTION

The Hamiltonian for the system is

$$\hat{H} = \frac{\hat{p}^2}{2m}$$

and the translational momentum is simply

$$p = \text{const} = p_0 \quad . \tag{4.1}$$

The equations for the amplitudes β_ℓ are

$$i\hbar\, \dot{\overline{\beta}}_\ell = \frac{\partial K}{\partial \beta_\ell} - \frac{\dot{q}}{b\sqrt{2}} \frac{\partial}{\partial \beta_\ell} (\chi + \overline{\chi}) \quad , \tag{4.2}$$

where (see (A.3))

$$K = \sum_{ij} \beta_i \overline{\beta}_j \langle z,i|\frac{\tilde{p}^2}{2m}|z,j\rangle \quad . \tag{4.3}$$

Or, explicitly, up to a global phase factor,

$$i\hbar\, \dot{\overline{\beta}}_\ell = \overline{\beta}_\ell \frac{\hbar^2 \ell}{2mb^2} - \frac{\hbar^2}{4mb^2}\left[\sqrt{(\ell+1)(\ell+2)}\ \overline{\beta}_{\ell+2} - \sqrt{\ell(\ell+1)}\ \overline{\beta}_{\ell-2}\right] + \theta(\beta^3). \tag{4.4}$$

Now, we want to describe the time development of a gaussian wave packet and this means that equations (4.4) must be solved with initial conditions $\overline{\beta}_i(0) = \delta_{i0}$. Besides, we are interested in the short time behaviour of a gaussian wave packet in which case the terms $\theta(\beta^3)$ in equation (4.4) may be dropped. In this case, the solutions of equation (4.4) are

$$\overline{\beta}_{2\ell+1}(t) = 0 \quad , \quad \forall \ell \; ,$$

$$\overline{\beta}_0(t) = 1 - \frac{\hbar^2 t^2}{16 m^2 b^4} \quad ,$$

$$\overline{\beta}_2(t) = \frac{i\hbar t}{2\sqrt{2}\, mb^2} + \frac{\hbar^2 t^2}{4\sqrt{2}\, m^2 b^2} + \theta(t^3) \quad ,$$

$$\overline{\beta}_{2\ell}(t) = \theta(t^2) \quad , \quad \text{for} \quad \ell \geq 2$$

and

$$q(t) = q_0 + \frac{p_0 t}{m} \quad . \tag{4.5}$$

(The last equation was obtained by solving (3.12) using (3.2a)).

The width of the wave packet at a time t is given by:

$$\langle\psi|q^2|\psi\rangle = \langle \underset{\sim}{z}|q^2|\underset{\sim}{z}\rangle = \frac{b^2}{2}\left[|\beta_0|^2 + 3|\beta_1|^2 + 5|\beta_2|^2 + \sqrt{2}\,(\beta_2+\bar{\beta}_2)\right] + \theta(t^3)$$

$$= \frac{b^2}{2}\left(1 + \frac{\hbar^2 t^2}{m^2 b^4}\right) + \theta(t^3) \qquad (4.6)$$

Thus, the result of the TDVP applied to the free motion of a gaussian wave packet is that for small time intervals it moves like a classical particle and spreads by a factor $\left(1 + \frac{\hbar^2 t^2}{m^2 b^4}\right)^{1/2}$ (see ref. 9) as predicted by quantum mechanics.

V. <u>GAUSSIAN WAVE PACKET INTERACTING WITH AN EXPONENTIAL BARRIER</u>

The Hamiltonian of the system is

$$H = \frac{\hat{p}^2}{2m} + V_0\, e^{\gamma\hat{q}}$$

and we shall solve numerically equations (3.12) and (3.18) (or (3.20)). In order to obtain a numerical solution it is necessary to truncate the system of equations. For small deformation, only a few terms should be sufficient. We shall consider terms β_n for $n \leq 3$. With this assumption, we obtain the following equations for q and p by using (3.2a) and (A.9) in (3.12)

$$\dot{q} = \frac{\partial H}{\partial p} \cong \frac{p}{m} + \frac{i\hbar}{2mb}\sum_{n=0}^{2}\sqrt{2(n+1)}\,(\beta_n\bar{\beta}_{n+1} - \bar{\beta}_n\beta_{n+1}) \ , \qquad (5.1a)$$

$$\dot{p} = -\frac{\partial H}{\partial q} \cong -|\beta_0|^2 U_0\gamma e^{\gamma q} - \sum_{n=1}^{3}\sum_{k=1}^{n}|\beta_n|^2 \frac{2^{n-k}(n-1)!}{(k-1)!k!}\left(\frac{b}{\sqrt{2}}\right)^{2k} U_0\gamma^{2k+1}e^{\gamma q} +$$

$$-\sum_{m>n=1}^{3}\sum_{k=0}^{n}(\beta_n\bar{\beta}_m + \beta_m\bar{\beta}_n)\frac{2^{n-k}(m-1)!\sqrt{n!}}{\sqrt{m!}\,(m-n+k-1)!k!}\left(\frac{b}{\sqrt{2}}\right)^{m-n+2k}\gamma^{m-n+2k+1}e^{\gamma q} \ , \qquad (5.1b)$$

where

$$U_0 = V_0\, e^{b^2\gamma} \ .$$

And the equations for β_n, $n \leq 3$, are obtained likewise by using (3.2a) and (A.9) in (3.20), the result being

$$\dot{\beta}_m = \frac{1}{i\hbar}\frac{\partial h}{\partial\beta_m} \cong \frac{1}{i\hbar}\sum_{n=0}^{3}\bar{\beta}_n S_{n\ell} \ , \qquad (5.1c)$$

where $S_{n\ell} = S_{\ell n}$ is given by

$$S_{nn} = \frac{\hbar^2}{4mb^2}(2n+1) + U_0 e^{\gamma q}\delta_{n0} + \sum_{k=1}^{n}\frac{2^{n-k}(n-1)!}{(k-1)!k!}\left(\frac{b}{\sqrt{2}}\right)^{2k} U_0\gamma^{2k}e^{\gamma q} \ ,$$

$$S_{n\ell} = -\frac{\hbar^2}{4mb^2}\sqrt{(\ell+1)(\ell+2)}\ \delta_{n,\ell+2} +$$

$$+\sum_{k=0}^{\ell}\frac{2^{\ell-k}(n-1)!\sqrt{\ell!}}{\sqrt{n!}\,(n-\ell+k-1)!k!}\left(\frac{b}{\sqrt{2}}\right)^{n-\ell+2k}\gamma^{n-\ell+2k}U_0 e^{\gamma q} \ , \quad n>\ell . \qquad (5.2)$$

It should be noted that the first term of the expression for $S_{n\ell}$ in (5.2) is responsible for the free spreading of the wave packet. As we want to investigate just the effect of the potential barrier on the wave packet, the numerical calculations were done without that term. And the results of the numerical calculation, with that term removed from (5.1), are exhibitted in figure 1 for $0 \leq t \leq 0.09$. Interference effects are observed near the classical turning point and small oscillations are observed even asymptotically due to phase factors,

$$\bar{\beta}_\ell (t \to \infty) = \text{const } e^{-\frac{i\hbar}{4mb^2}(2\ell+1)t} \qquad (5.3)$$

The final values of $|\beta_n|^2$ are

$$|\beta_0|^2 = 0.974$$

$$|\beta_1|^2 = 1.46\ 10^{-4}$$

$$|\beta_2|^2 = 7.67\ 10^{-3}$$

$$|\beta_3|^2 = 0.0196$$

$$\sum_{n=0}^{3} |\beta_n|^2 = 1.00 \quad .$$

VI. CONCLUSIONS

We have analized the time evolution of a gaussian wave packet in the framework of the time dependent variational principle with parametrized trial function. It is a simple example but illustrates well the method. We considered two cases: free motion and interaction with a potential barrier.

The choice of parametrization of the trial wave function is determined by the particular physical aspects of the system which is to be studied. The parametrization appropriate for describing the shape evolution of the wave packet during its motion was shown to be a natural generalization of the parametrization used in describing the ellastic scattering of two particles.

In the case of free motion we have shown that the TDVP gives the quantum mechanical results, for small time intervals t: the center of the packet moves like a classical particle and it spreads linearly in t.

In the case of the gaussian wave packet interacting with a barrier (we considered an exponential barrier) we obtained interference of waves with different momenta when the center of the packet approaches the classical turning point.

APPENDIX

Here we shall calculate explicitly the expectation value of the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q}) \qquad (A.1)$$

in the states $|\underset{\sim}{z}\rangle$:

$$H = \langle \underset{\sim}{z}|\hat{H}|\underset{\sim}{z}\rangle = \sum_{m,n} \bar{\beta}_m \beta_n \langle z,n|\frac{\hat{p}^2}{2m} + V(\hat{q})\,|z,m\rangle \quad , \qquad (A.2)$$

where we have defined

$$|z,\ell\rangle = e^{\bar{z}\hat{a}^\dagger} e^{-z\hat{a}}|\ell\rangle \quad . \qquad (A.3)$$

The calculation of the kinetic term is rather simple if we write $\hat{p}$ in terms of the creation and aniquilation operators and note that

$$\hat{a}^2|z,n\rangle = \sqrt{n(n+1)}\,|z,n-2\rangle + 2\bar{z}\sqrt{n}\,|z,n-1\rangle + \bar{z}^2|z,n\rangle \qquad (A.4a)$$

$$\hat{a}^{\dagger 2}|z,n\rangle = \sqrt{(n+1)(n+2)}\,|z,n+2\rangle + 2z\sqrt{n+1}\,|z,n+1\rangle + z^2|z,n\rangle \qquad (A.4b)$$

$$\hat{a}^\dagger\hat{a}|z,n\rangle = (n+z\bar{z})|z,n\rangle + z\sqrt{n}\,|z,n-1\rangle + \bar{z}\sqrt{n+1}\,|z,n+1\rangle \quad . \qquad (A.4c)$$

So, we find

$$K_{nm} = \langle z,n|\frac{\hat{p}^2}{2m}|z,m\rangle = -\frac{\hbar^2}{4mb^2}\Big\{\Big[(z-\bar{z})^2 - (2n+1)\Big]\,\delta_{n,m} + \sqrt{m(n-1)}\,\delta_{n,m-2} +$$

$$+ \sqrt{(m+1)(n+2)}\,\delta_{n,m+2} - 2\sqrt{m}\,(z-\bar{z})\,\delta_{n,m-1} + 2\sqrt{n+1}\,(z-\bar{z})\,\delta_{n,m+1}\Big\} . \qquad (A.5)$$

Before calculate the matrix elements for the potential we notice that:

$$1)\quad |z,n\rangle = e^{\bar{z}\hat{a}^\dagger} e^{-z\hat{a}}|n\rangle = e^{\bar{z}\hat{a}^\dagger}(1 - z\hat{a} + \ldots)|n\rangle$$

$$= \frac{e^{\bar{z}\hat{a}^\dagger}}{\sqrt{n!}}\,(\hat{a}^\dagger - n\,z\,\hat{a}^{\dagger n-1} + \ldots)$$

$$= \frac{1}{\sqrt{n!}}\,(\hat{a}^\dagger - z)^n\,|z,0\rangle \quad , \qquad (A.6)$$

and

$$2)\quad \Big[V(\hat{q}),\hat{a}^{\dagger n}\Big] = +\frac{b}{\sqrt{2}}\Big(2\hat{a}^\dagger + \frac{b}{\sqrt{2}}\frac{\partial}{\partial\hat{q}}\Big)^{n-1}\frac{\partial V(\hat{q})}{\partial\hat{q}} \qquad (A.7)$$

where the $\hat{a}^\dagger$'s must be always put on the left when the binomion is calculated. This last result can be demonstrated by induction from

$$\Big[V(\hat{q}),\hat{a}^\dagger\Big] = \frac{b}{\sqrt{2}}\frac{\partial V}{\partial q} \quad .$$

Using these two relations and considering $m > 0$ and $m \geqslant n$ we get

$$v_{nm}(q) \equiv \langle z,n|V(\hat{q})\,|z,m\rangle = \frac{1}{\sqrt{n!m!}}\,\langle z,0|\,(\hat{a}-\bar{z})^n\,V(\hat{q})\,(\hat{a}^\dagger-z)^m\,|z,0\rangle$$

$$= \frac{1}{\sqrt{n!m!}}\Big[\langle z,0|\,(\hat{a}-\bar{z})^n\,(\hat{a}^\dagger-z)^m\,V(\hat{q})\,|z,0\rangle + \langle z,0|\,(a-z)^n\Big[V,(\hat{a}^\dagger-z)^m\Big]|z,0\rangle\Big] \quad .$$

For $m \geqslant n$, the first term gives simply

$$\langle z,0|V(\hat{q})\,|z,0\rangle\,\delta_{m,n} \quad .$$

The second one may also be calculated and the final result is (after some algebra)

$$v_{nm}(q) = \begin{cases} \sum\limits_{k=0}^{n} \dfrac{2^{n-k}(m-1)!\sqrt{n!}}{\sqrt{m!}\,(m-n+k-1)!\,k!} \left(\dfrac{b}{\sqrt{2}}\right)^{m-n+2k} \langle z,0| \dfrac{\partial^{m-n+2k} V(\bar{q})}{\partial \bar{q}^{m-n+2k}} |z,0\rangle & \text{if } m > n \\ \\ \langle z,0|V|z,0\rangle + \sum\limits_{k=1}^{n} \dfrac{2^{n-k}(n-1)!}{(k-1)!\,k!} \left(\dfrac{b}{\sqrt{2}}\right)^{2k} \langle z,0| \dfrac{\partial^{2k} V(\bar{q})}{\partial \bar{q}^{2k}} |z,0\rangle & \text{if } m = n \end{cases} \tag{A.8}$$

and

$$H = \sum_{m,n} \bar{\beta}_m \beta_n (K_{nm} + v_{nm})$$

$$\begin{aligned} H = \frac{h^2}{4mb^2} \Bigg[& -(z-\bar{z})^2 - \sum_{n=0} (\beta_n \bar{\beta}_{n+2} + \bar{\beta}_n \beta_{n+2}) \sqrt{(n-1)(n+2)} \\ & - 2 \sum_{n=0} (z-\bar{z}) (\bar{\beta}_n \beta_{n+1} - \beta_n \bar{\beta}_{n+1}) \sqrt{n+1} + \\ & + \sum_{n=0} |\beta_n|^2 (2n+1) \Bigg] + |\beta_0|^2 e^{-z\bar{z}} \langle z,0|V(q)|z,0\rangle + \\ & + \sum_{n=1} \sum_{k=1}^{n} |\beta_n|^2 \frac{2^{n-k}(n-1)!}{(k-1)!\,k!} \left(\frac{b}{\sqrt{2}}\right)^{2K} \langle z,0| \frac{\partial^{2k} V}{\partial q^{2k}} |z,0\rangle + \\ & + \sum_{m>n=0} (\beta_n \bar{\beta}_m + \beta_m \bar{\beta}_n) \sum_{k=0}^{n} \frac{2^{n-k}(m-1)!\sqrt{n!}}{\sqrt{m!}\,(m-n+k-1)!\,k!} \left(\frac{b}{\sqrt{2}}\right)^{m-n+2k} \langle z,0| \frac{\partial^{m-n+2k} V}{\partial q^{m-n+2k}} |z,0\rangle . \end{aligned} \tag{A.9}$$

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FIGURE CAPTION

FIG. 1 - Time evolution of the shape of the wave packet interacting with an exponential barrier. The parameters used in the numerical calculation are: $m = 0.5$, $b = 0.3$, $\gamma = 0.1$ and $V_0 = 50$.

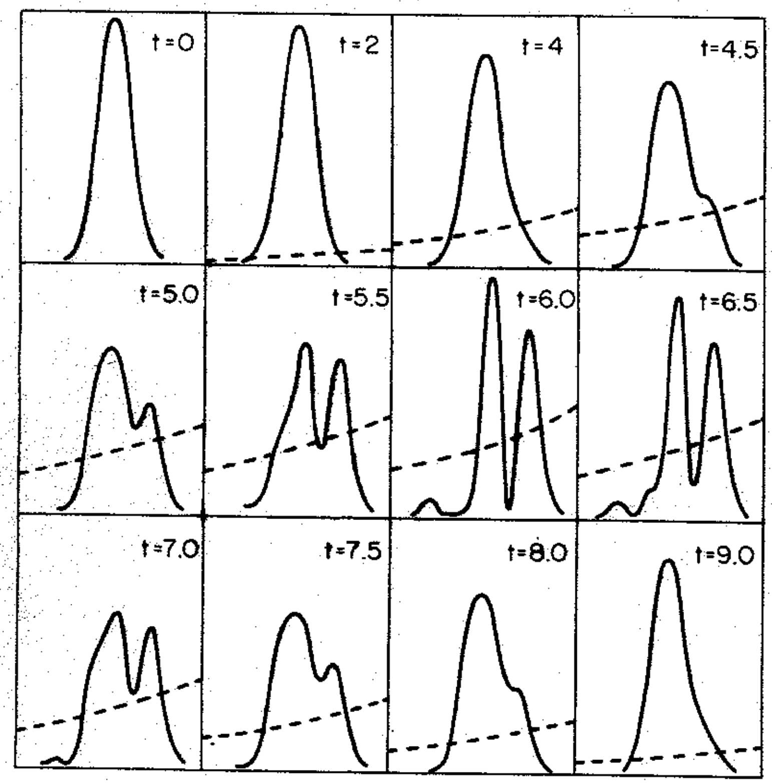

FIGURE 1