Chemical Physics 91 (1984) 27–34
North-Holland, Amsterdam

A SEMICLASSICAL JUSTIFICATION FOR THE USE OF NON-SPREADING WAVEPACKETS IN DYNAMICS CALCULATIONS

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Received 30 March 1984

A justification is given for the use of non-spreading or frozen gaussian packets in dynamics calculations. In this work an initial wavefunction or quantum density operator is expanded in a complete set of gaussian wavepackets. It is demonstrated that the time evolution of this wavepacket expansion for the quantum wavefunction or density is correctly given within the approximations employed by the classical propagation of the average position and momentum of each gaussian packet, holding the shape of these individual gaussians fixed. The semiclassical approximation is employed for the quantum propagator and the stationary phase approximation for certain integrals is utilized in this derivation. This analysis demonstrates that the divergence of the classical trajectories associated with the individual gaussian packets accounts for the changes in shape of the quantum wavefunction or density, as has been suggested on intuitive grounds by Heller. The method should be exact for quadratic potentials, and this is verified by explicitly applying it for the harmonic oscillator example.

1. Introduction

This manuscript considers the spreading or non-spreading of wavepackets. On one hand molecular dynamics simulations have given useful results for many properties of bulk systems. These simulations are based upon classical mechanics and would seem to indicate that some localized wavepacket description for the particle wavefunctions must be applicable on the time scales of interest. Otherwise the use of classical mechanics would appear to be inappropriate.

On the other hand, a simple estimate of the packet spreading for a one-dimensional argon atom, for instance, indicates that the localized packet picture is applicable only for very short times. For a rough estimate we use the well-known result for a free particle gaussian wavepacket [1]. Taking the initial wavefunction to be

$$\psi(x, 0) = (2\alpha/\pi)^{1/4} \exp\left[-\alpha(x - x_0)^2 + i p_0 (x - x_0)\right]. \tag{1}$$

At later times, $\psi(x, t)$ retains its gaussian form but α in the exponential is replaced by

$$\alpha_t = \alpha(1 + 2i\alpha t/m)^{-1} \tag{2}$$

and a new prefactor appears. The width of the wavefunction (in position) is determined by the real part of α_t, which goes as

$$\mathrm{Re}\ \alpha_t = \alpha(1 + 4\alpha^2 t^2/m^2)^{-1} = \alpha(1 + \beta_t \alpha^2)^{-1}. \tag{3}$$

In atomic units the mass of argon is ≈ 72000 and one picosecond is ≈ 40000 au. Therefore $\beta_t \equiv 4t^2/m^2 \approx 1.1$. The maximum value of Re α_t (which corresponds to the minimum width) as a function of α is obtained when $\alpha^2 = 1/\beta_t$. The conclusion is that an initially gaussian packet must spread over a width of at least $\sigma_t = (4\ \mathrm{Re}\ \alpha_t)^{-1/2} \approx 0.75$ au on a picosecond time scale.

0301-0104/84/$03.00

Certainly the potentials of interest in a liquid change considerably over this distance. It is true that the free particle is not a very good model for a particle in a condensed medium. However, the general point that packets do not remain localized for times of many picoseconds seems likely to be valid. The harmonic oscillator is a notable exception to the phenomena of packet spreading. In this case the packet remains localized if the width of the packet matches that of the harmonic oscillator ground state. Even if its width differs from that of the ground state, the wavepacket refocuses once a period. Recent numerical studies [2–4] on anharmonic potentials indicate recurrences on the order of many vibrational periods. These studies also show relatively long stretches of time where the particle density is quite delocalized.

This brings us back to the question, if the wavepackets become delocalized after relatively short periods of time, how can molecular dynamics studies (or any type of classical analysis) be meaningful? The answer we propose is that while a single localized wavepacket whose average position and momentum obey classical equations does not accurately approximate a quantum system, a set of localized packets can. The diverging of the trajectories executed by the average packet position and momentum accurately mimics the quantum delocalization. This is essentially the heuristic justification that Heller [5] has recently proposed for a method he calls the frozen gaussian approximation.

This method amounts to expanding a wavefunction in terms of a set of gaussians, and then propagating these gaussians with fixed shape according to the laws of classical mechanics.

In this paper we provide a mathematic justification of this method. The approximations involved in this derivation are the use of the semiclassical approximation for the Feynman propagator [6] and the stationary phase approximation for various integrations [7].

2. Theory

Suppose we propagate some initial wavefunction $\psi_0(r)$ forward in time

$$\psi(r, t) = \int \mathrm{d}r_0 \, K(r, r_0; t)\psi_0(r_0), \tag{4}$$

where $K(r, r_0; t)$ is the Feynman propagator [6]. The set of gaussians

$$g(r; r_1, p_1; \gamma) = (2\gamma/\pi)^{1/4} \exp\left[-\gamma(r - r_1)^2 + \mathrm{i}p_1 \cdot (r - r_1)\right], \tag{5}$$

form an over complete set for any real $\gamma > 0$ [8–10]. In terms of these functions the resolution of the identity is

$$\delta(r - r') = (2\pi)^{-N} \int \mathrm{d}r_1 \int \mathrm{d}p_1 \, g(r; r_1, p_1; \gamma) g^*(r'; r_1, p_1; \gamma). \tag{6}$$

where N is the dimensionality of the vectors r, r_0; r_1 and p_1. The constant $\hbar$ has been set to unity for convenience. Inserting (6) into (4) twice yields

$$\begin{aligned}\psi(r, t) = (2\pi)^{-2N} \int_{-\infty}^{\infty} \mathrm{d}r_0 \int_{-\infty}^{\infty} \mathrm{d}r_i \int_{-\infty}^{\infty} \mathrm{d}r_f \int_{-\infty}^{\infty} \mathrm{d}r_1 \int_{-\infty}^{\infty} \mathrm{d}p_1 \int_{-\infty}^{\infty} \mathrm{d}r_2 \int_{-\infty}^{\infty} \mathrm{d}p_2 \, g(r; r_2, p_2; \gamma) \\ \times g^*(r_f; r_2, p_2; \gamma) K(r_f r_i; t) g(r_i; r_1, p_1; \gamma) g^*(r_0; r_1, p_1; \gamma) \psi_0(r_0),\end{aligned} \tag{7}$$

where all the integrations have been explicitly written out for emphasis. At this point it is convenient to replace the quantum propagator by its semiclassical approximation

$$K(r_f, r_i; t) = \left[\left|-\partial^2 S/\partial r_i \partial r_f\right|/(2\pi \mathrm{i})^N\right]^{1/2} \exp\{\mathrm{i}S\} \equiv A \exp\{\mathrm{i}S\}, \tag{8}$$

where S is the action for a classical trajectory connecting r_i and r_f in time t. That is,

$$S(r_f, r_i; t) = \int L \, dt, \tag{9}$$

where L is the lagrangian, $T - V$. $|\partial^2 S/\partial r_i \partial r_f|$ is the determinant of the second derivative matrix. Substitution from (5) and (8) into (7) produces

$$\psi(r, t) = (2\pi)^{-2N}(2\gamma/\pi)^N \int dr_i \int dr_f \int dr_0 \int dr_1 \int dp_1 \int dr_2 \int dp_2 A \, e^{\phi} \psi_0(r_0), \tag{10}$$

where A is the prefactor in (8) and

$$\begin{aligned}\phi = &-\gamma(r - r_2)^2 + i p_2 \cdot (r - r_2) - \gamma(r_f - r_2)^2 - i p_2 \cdot (r_f - r_2) \\ &+ iS(r_f, r_i; t) - \gamma(r_i - r_1)^2 + i p_1 \cdot (r_i - r_1) - \gamma(r_0 - r_1)^2 - i p_1 \cdot (r_0 - r_1).\end{aligned} \tag{11}$$

We now alter the integration path associated with p_1 so that

$$p_1 = q_1 - 2i\gamma r_1. \tag{12}$$

This merely replaces the integration of each component of p_1 along the real axis by an integration along a parallel path that has been displaced from the real axis by 2γ times the value of the corresponding component of r_1. Likewise we replace p_2 by

$$p_2 = q_2 + 2i\gamma r_2 \tag{13}$$

and each component of q_2 is integrated over the entire real axis. We now perform the r_1, r_2, r_i and r_f integrations by stationary phase holding r_0, q_1 and q_2 fixed. The resulting stationary phase conditions are

$$\begin{aligned}&\partial\phi/\partial r_1 = -4\gamma(r_1 - r_i) = 0, \qquad \partial\phi/\partial r_2 = -4\gamma(r_2 - r_f) = 0, \\ &\partial\phi/\partial r_i = i(p_1 + \partial S/\partial r_i) - 2\gamma(r_i - r_1) = 0, \qquad \partial\phi/\partial r_f = -i(p_2 - \partial S/\partial r_f) - 2\gamma(r_f - r_2) = 0.\end{aligned} \tag{14}$$

Recall that $\partial S/\partial r_f \equiv p_f$ is the final momentum of the classical trajectory which begins at r_i and ends at r_f at time t later. Likewise $\partial S/\partial r_i \equiv -P_i$ is the initial momentum of this trajectory. The resulting wavefunction after the stationary phase integrations has the form

$$\begin{aligned}\psi(r_1, t) = (2\pi)^{-2N}(2\gamma/\pi)^N \int_{-\infty}^{\infty} dr_0 \int_{-\infty}^{\infty} dq_1 \int_{-\infty}^{\infty} dq_2 \, A\left[(2\pi)^{4N}/D\right]^{1/2} \\ \times \exp\left[-\gamma(r - R_f)^2 + i P_f \cdot (r - R_f) + iS(R_i, R_f; t) - \gamma(r_0 - R_i)^2 - i P_i \cdot (r_0 - R_i)\right] \psi_0(r_0),\end{aligned} \tag{15}$$

where R_i, R_f, P_i and P_f are considered functions of q_1, q_2 and t. Eqs. (12)–(14) imply that they are the initial and final positions and momenta for a (complex) trajectory which obeys the conditions

$$q_1 = P_i + 2i\gamma R_i \tag{16}$$

and

$$q_2 = P_f - 2i\gamma R_f. \tag{17}$$

In (15) D is the determinant made of second derivatives of ϕ with respect to r_i, r_f, r_1 and r_2

$$D \equiv \left| \frac{\partial^2 \phi}{\partial^2 (r_i, r_f, r_1, r_2)} \right| = (4\gamma i)^{2N} \begin{vmatrix} \partial^2 S/\partial r_i^2 - 2\gamma i \mathbf{l} & \partial^2 S/\partial r_i \partial r_f \\ \partial^2 S/\partial r_f \partial r_i & \partial^2 S/\partial r_f^2 - 2\gamma i \mathbf{l} \end{vmatrix}. \tag{18}$$

where I stands for N-dimensional identity matrix. These second derivatives are evaluated with r, r_0, q_1, q_2 and t held constant; eqs. (12) and (13) must be employed to account for the r_1 and r_2 dependence of p_1 and p_2, and S is treated as a function of r_i, r_f and t. If more than one trajectory satisfies conditions (16) and (17), the contributions of each of these should be summed.

Eqs. (16) and (17) specify P_i, R_i, P_f and R_f in terms of the integration variables q_1 and q_2 [along with the condition that a *classical* trajectory of duration t connect the phase space points (R_i, P_i) and (R_f, P_f)]. The independent variables can be changed to R_i and P_i. This change of variables gives

$$\psi(r,t) = (2\gamma/\pi)^N (1/2\pi)^{2N} \int_{-\infty}^{\infty} dr_0 \int_{-\infty}^{\infty} dR_i \int_{-\infty}^{\infty} dP_i JA\left[(2\pi)^{4N}/D\right]^{1/2} \times \exp\left[-\gamma(r-R_f)^2 + iP_f\cdot(r-R_f) + iS(R_i,R_f;t) - \gamma(r_0-R_i)^2 - iP_i\cdot(r_0-R_i)\right]\psi_0(r_0). \tag{19}$$

where J is the jacobian of the transformation

$$J = \left|\begin{matrix} \partial q_1/\partial R_i & \partial q_2/\partial R_i \\ \partial q_1/\partial P_i & \partial q_2/\partial P_i \end{matrix}\right| = (2\gamma i)^N \left|\left(\frac{\partial P_f}{\partial P_i} + \frac{i}{2\gamma}\frac{\partial P_f}{\partial R_i}\right) - 2\gamma i\left(\frac{\partial R_f}{\partial P_i} + \frac{i}{2\gamma}\frac{\partial R_f}{\partial R_i}\right)\right|. \tag{20}$$

Eq. (19) can be rewritten as

$$\psi(r,t) = (2\gamma/\pi)^{N/2} \int_{-\infty}^{\infty} dR_i \int_{-\infty}^{\infty} dP_i JAD^{-1/2} g(r; R_f, P_f; \gamma) \times \exp\left[iS(R_i,R_f;t)\right] \int_{-\infty}^{\infty} dr_0\, g^*(r_0; R_i, P_i; \gamma)\psi_0(r_0). \tag{21}$$

R_f and P_f are considered functions of R_i, P_i and t.

Eq. (21) is the main result of the paper. When $t_f \to t_i$, then $g(r; R_f, P_f; \gamma) \to g(r; R_i, P_i; \gamma)$ and a little work reveals that $(2\gamma/\pi)^{N/2} JAD^{-1/2} \to (2\pi)^{-N}$. In this case eq. (21) is merely the expansion of ψ_0 in the overcomplete set $g(r; R_i, P_i; \gamma)$. More generally eq. (21) states that within the approximations employed the time evolution of $\psi(r,t)$ is given by propagating the average position and momentum of each member of this overcomplete set according to classical mechanics and holding its width fixed. The resulting gaussian $g(r; R_f, P_f; \gamma)$ is multiplied by the phase factor $\exp(iS)$, the prefactor $(2\gamma/\pi)^{N/2} JAD^{-1/2}$ and the coefficient from the $t = 0$ expansion $\int dr_0\, g^*(r_0; R_i, P_i; \gamma)\psi_0(r_0)$.

Since conditions (16) and (17) specify complex values of P_i and R_i, the contour of integration in (19) wanders over the complex plane. However, in changing integration variables from q_1 and q_2 to R_i and P_i, we have implicitly deformed this contour so that the integration in (21) is over real values of R_i and P_i.

A strict justification that this deformation of the integration path does not alter the value of the integral would require a detailed knowledge of the analytical structure of the potential energy function in order to prove that the classical action $S(R_i, R_f, t)$ is analytical throughout the region over which the contour is deformed. It is also necessary to show that the integrand tends to zero rapidly enough at the ends on the contour. This can in fact be accomplished for specific potential functions such as a quadratic potential.

The stationary phase approximation, however, assumes that only the behavior of the integrand near the stationary phase points is important. As long as the variable transformations preserve the location of these points, the value of the integral is unaltered in this approximation.

Since

$$\frac{\partial\phi}{\partial R_i} = \frac{\partial q_i}{\partial R_i}\frac{\partial\phi}{\partial q_i} + \frac{\partial q_f}{\partial R_i}\frac{\partial\phi}{\partial q_f} \quad \text{and} \quad \frac{\partial\phi}{\partial P_i} = \frac{\partial q_i}{\partial P_i}\frac{\partial\phi}{\partial q_i} + \frac{\partial q_f}{\partial P_i}\frac{\partial\phi}{\partial q_f}, \tag{22}$$

points that obey the conditions $\partial\phi/\partial q_i = \partial\phi/\partial q_f = 0$, also obey the conditions $\partial\phi/\partial R_i = \partial\phi/\partial P_i = 0$. There still is the possibility of introducing additional stationary phase points where $\partial\phi/\partial q_i = \partial q_f/\partial R_i = \partial q_f/\partial q_i = 0$ but $\partial\phi/\partial q_f \neq 0$. However these should occur at most for isolated values of r_0 and r since the $3N$ conditions $\partial\phi/\partial q_i = \partial q_f/\partial R_i = \partial q_f/\partial P_i = 0$ form an overdetermined set of equations for the $2N$ unknowns (R_i, P_i). As long as these conditions are satisfied for values of r and r_0 that at most constitute a set of measure zero, they will make no contribution to $\psi(r, t)$.

3. Discussion

We have demonstrated in this paper that when a wavefunction is expanded in a complete set of gaussian wavepackets, the diverging or converging of the positions of the centers of these packets in phase space, as given by classical mechanics, accounts for the spreading or focusing of the original wavefunctions (within the semiclassical approximation for the propagator and the stationary phase approximation for the integrations involved). The effects of quantum-mechanical changes in shape as the individual gaussians propagate in time totally cancel within these approximations and the frozen gaussian approximation is justified.

So far nothing has been said about the parameter γ, which determines the width of the gaussian in positions and momentum space. Since the set of gaussians is overcomplete for all values of γ, this parameter is completely arbitrary from a formal point of view. However, its choice may be important numerically, when the continuous representation of the overcomplete set of gaussians is approximated by some finite discrete set. The integrand in (19) is an oscillatory function of R_i and P_i. If a very large value of γ is chosen, then a wide range of P_i should contribute to the integral. This will include initial momenta corresponding to high-energy trajectories, where the integrand is likely to be oscillating rapidly, since S contains the integral over the kinetic energy which involves the square of the momentum. This could cause convergence problems. Heller has studied the use of finite sets of gaussians [5,11].

The classical propagator is exact for potentials that contain no higher than quadratic terms [6]. In this case the action is at most a quadratic function, and therefore the stationary phase approximation for the integrations is exact. Consequently, the frozen gaussian approximation is exact for potentials containing at most quadratic terms, such as the free particle and harmonic oscillator potentials. We specifically used this fact to algebraically check our analysis for the harmonic oscillator (see appendix). Since semiclassical approximations are generally exact for this class of potentials, this result is not overly startling. However, the corollary that the quantum effects due to oscillations in the widths of the individual gaussians exactly and completely cancel is not an obvious result.

The results of this paper have been presented for the propagation of an initial wavefunction. The same arguments apply if the initial wavefunction $\psi_0(r_0)$ is replaced by a density operator $\hat{\rho}$. In this case eq. (21) takes the form

$$\rho(r, r'; t) = (2\gamma/\pi)^{N/2}(1/2\pi)^N \int dR_i \int dP_i \int dR_a \int dP_a JAD^{-1/2} g(r; R_f, P_f; \gamma)$$
$$\times \exp[iS(R_f, R_i; t)] \int dr_0' \int dr_0 g^*(r_0; R_i, P_i; \gamma)\rho_0(r_0, r_0')$$
$$\times g(r_0'; R_a, P_a; \gamma)\, g^*(r'; R_a, P_a; \gamma). \tag{23}$$

The matrix element $\int dr_0 \int dr_0' g^*(r_0; R_i, P_i; \gamma)\rho_0(r_0, r_0')g(r_0'; R_a, P_a; \gamma)$ involves integration over the variables r_0 and r_0'. The final positions and momenta, R_f and P_f, respectively, are functions of R_i, P_i and t, as above. If ρ_0 is the canonical density function $e^{-\beta H}/\mathrm{Tr}\, e^{-\beta H}$, then an approximation can be developed for

$\int d\mathbf{r}_0' \int d\mathbf{r}_0 g^*(\mathbf{r}_0; \mathbf{R}_i, \mathbf{P}_i; \gamma)\rho_0(\mathbf{r}_0, \mathbf{r}_0') g(\mathbf{r}_0', \mathbf{R}_a, \mathbf{P}_a; \gamma)$ which is analogous to the one which is derived for $\int d\mathbf{r}_f \int d\mathbf{r}_i g^*(\mathbf{r}_f; \mathbf{r}_2, \mathbf{p}_2; \gamma) K(\mathbf{r}_f, \mathbf{r}_i; t) g(\mathbf{r}_i; \mathbf{r}_1, \mathbf{p}_1; \gamma)$ in this paper, since $K = e^{iHt}$. This correspondence between the real time propagator and the canonical density function is well known [6,7,12,13], and we do not work through the details here.

Quite a few years ago Klauder presented a series of papers [9,10] discussing continuous representations of quantum mechanics, of which the gaussian representation employed herein is a specific example. In Klauder's work classical mechanics is shown to result from quantum mechanics in the limit that the basis vectors in the representations (the individual gaussians in our continuous set) are maped into other basis vectors in the set. As a consequence, classical mechanics may be considered exact to the extend that gaussian functions of a specific width remain gaussian and retain the same width as a function of time. Klauder's work has recently served as the motivation of a rigid wavepacket dynamics calculation [14]. Our result suggests that the situation is often much more favorable than Klauder's analysis indicates, since much of the effect of spreading and changing of shape of the basis vectors in fact cancels.

Acknowledgement

This work is supported by NSF Grant CHE-8219380.

Appendix

It must be admitted that the exactness of the wavepacket expansion (21) in terms of frozen gaussians for at most quadratic potentials comes out as a bit of a surprise. That is why in this appendix it is shown how to recover from the expansion (21) Heller's expressions [15] for propagation of initially gaussian wavepackets (1) for a harmonic oscillator and a free particle of mass m, which are exact in these cases. Basically there is shown a sketch of calculations for a harmonic oscillator. However it is arranged in such a way that at any step a free particle case is recovered by taking the limit of harmonic oscillator frequency $\omega \to 0$.

For a one-dimensional harmonic oscillator the formula (21) can be recast in the following way

$$\psi(x,t) = (2\gamma/\pi)(2\alpha/\pi)^{1/4} \int_{-\infty}^{\infty} dx_i \int_{-\infty}^{\infty} dp_i \int_{-\infty}^{\infty} dx_0 \, JAD^{-1/2} e^{\phi}, \tag{24}$$

where

$$\phi = -\gamma(x - x_f)^2 + i p_f (x - x_f) + (im\omega/2 \sin \omega t)\left[x_f^2 + x_i^2 \cos \omega t - 2x_f x_i\right]$$
$$-\gamma(x_0 - x_i)^2 - i p_i (x_0 - x_i) - \alpha(x_0 - \bar{x})^2 + i\bar{p}(x_0 - \bar{x}) \tag{25}$$

and x, x_f, p_f, x_i, p_i and x_0 are one-dimensional equivalents of $\mathbf{r}$, $\mathbf{R}_f$, $\mathbf{P}_f$, $\mathbf{R}_i$, $\mathbf{P}_i$ and $\mathbf{r}_0$ respectively, whereas $\bar{x}$, $\bar{p}$ are position and momentum of the initial wavepacket and α is the width of the initial packet.

Making use of formulae (8), (18) and (20) as well as the obvious transformation

$$x_f = x_i \cos \omega t + (p_i/m\omega) \sin \omega t, \qquad p_f = -x_i m\omega \sin \omega t + p_i \cos \omega t, \tag{26}$$

it is found after a bit of work that

$$A = (m\omega/2\pi i \sin \omega t)^{1/2}, \qquad D = i(4\gamma)^3 m\omega Z/\sin \omega t, \qquad J = 4i\gamma Z,$$

where

$$Z = \cos \omega t - \tfrac{1}{2} i(2\gamma/m\omega + m\omega/2\gamma) \sin \omega t. \tag{27}$$

Applying stationary phase integration (which is exact here since ϕ is quadratic and the prefactor is constant) to the variables x_i, p_i in the integral (24), the following equations for a stationary point are obtained

$$\partial\phi/\partial x_i = (2\gamma\cos\omega t - im\omega\sin\omega t)(x - x_t) + 2\gamma(x_0 - x_i) = 0,$$
$$\partial\phi/\partial p_i = [(2\gamma/m\omega)\sin\omega t + i\cos\omega t](x - x_t) - (x_0 - x_i) = 0, \tag{28}$$

so, the stationary point is given by

$$x_i = x_0, \qquad p_i = (m\omega/\sin\omega t)(x - x_0\cos\omega t). \tag{28a}$$

The second derivatives of ϕ, which are needed to obtain a prefactor for stationary phase integration, turn out to be

$$\partial^2\phi/\partial x_i^2 = -2\gamma(1 + \cos^2\omega t) + im\omega\sin\omega t\cos\omega t,$$
$$\partial^2\phi/\partial p_i^2 = -(1/m\omega)\sin\omega t[(2\gamma/m\omega)\sin\omega t + i\cos\omega t],$$
$$\partial^2\phi/\partial x_i\partial p_i = \partial^2\phi/\partial p_i\partial x_i = [(-2\gamma\cos\omega t + im\omega\sin\omega t)/m\omega]\sin\omega t \tag{29}$$

and the mentioned prefactor itself is given by

$$B = \frac{2\pi}{\left(-|\partial^2\phi/\partial(x_i, p_i)|\right)^{1/2}} = 2\pi[(4\gamma im\omega)\sin\omega t]^{-1/2}Z^{-1/2}. \tag{29a}$$

At this point it is worthwhile to notice that if the product

$$AJD^{-1/2}B = (1/4\gamma)(2\pi im\omega/\sin\omega t)^{1/2} \tag{30}$$

is inserted into the wavepacket (24) the parameter γ, which characterizes a set of frozen gaussians, disappears as it should be.

Inserting the stationary point (28a) into the phase (2) we get a new phase $\bar{\phi}$ for integration over x_0

$$\bar{\phi} = -\alpha(x_0 - \bar{x}) + i\bar{p}(x_0 - \bar{x}) + (im\omega/2\sin\omega t)[(x^2 + x_0^2)\cos\omega t - 2xx_0]. \tag{31}$$

Making use of stationary phase integration with respect to the variable x_0 in (24) the following stationary phase condition is found

$$\partial\bar{\phi}/\partial x_0 = -2\alpha(x_0 - \bar{x}) + i\bar{p} + (im\omega/\sin\omega t)(x_0\cos\omega t - x) = 0, \tag{32}$$

with the stationary point

$$x_0 = \frac{2\alpha\bar{x} + i\bar{p} - (im\omega/\sin\omega t)x}{2\alpha - (im\omega/\sin\omega t)\cos\omega t} \tag{32a}$$

and the prefactor

$$C = \left(\frac{-2\pi}{\partial^2\bar{\phi}/\partial x_0^2}\right)^{1/2} = 2\pi[2\alpha - (im\omega/\sin\omega t)\cos\omega t]^{1/2}. \tag{32b}$$

To recover Heller's exact form for the wavepacket (24) we have to find the phase $\bar{\phi}$ at the stationary point (32a) as a function of x_t, p_t, which are the current position and momentum of the wavepacket, rather than $\bar{x}$, $\bar{p}$ which are initial position and momentum respectively. This can be done with help of the reverse transformation (26) which expresses $\bar{x}$, $\bar{p}$ in terms of x_t, p_t. If the stationary point (32a) and the

abovementioned reversed transformation are inserted into (31), the phase $\bar{\phi}$ becomes a quadratic form of x, x_t and p_t.

A systematic way to show that $\bar{\phi}(x, x_t, p_t)$ has the proper form is to notice that $\bar{\phi}$ contains the classical action term $iS(x_t, \bar{x}(x_t, p_t))$. So if this term is subtracted from $\bar{\phi}(x, x_t, p_t)$, the remaining part

$$\Delta\bar{\phi} = \bar{\phi}(x, x_t, p_t) - iS(x_t, \bar{x}(x_t, P_t)) \tag{33}$$

must have a simple quadratic form of the following shape

$$\Delta\bar{\phi} = -\alpha(t)(x - x_t)^2 + ip_t(x - x_t). \tag{33a}$$

And indeed if we try to find the coefficients of x^2, xx_t, x_t^2, $p_t x$ and $p_t x_t$ in $\Delta\bar{\phi}$ it is not difficult but rather cumbersome to show that they are $\alpha(t)$, $-2\alpha(t)$, $\alpha(t)$, i and $-i$ respectively, where

$$\alpha(t) = \frac{m\omega}{2}\frac{(2\alpha/m\omega)\cot\omega t + i}{\cot\omega t + i(2\alpha/m\omega)} = \frac{1}{2}\frac{2\alpha\cos\omega t + im\omega\sin\omega t}{\cos\omega t + i[(2\alpha/m\omega)\sin\omega t]} \tag{34}$$

and it is related to Heller's $\alpha_H(t)$ by the identity $\alpha_H(t) = i\alpha(t)$.

Finally using eqs. (24), (30), (32b), (33) and (33a) the Heller's-type wavepacket for a harmonic oscillator, which is exact, is recovered. It reads

$$\psi(x, t) = (2\alpha/\pi)^{1/4}\exp\Big\{-\alpha(t)(x - x_t)^2 + ip_t(x - x_t) + iS(x_t, \bar{x}(x_t, p_t)) - \tfrac{1}{2}\ln[\cos\omega t + (2i\alpha/m\omega)\sin\omega t]\Big\}. \tag{35}$$

In the imit of $\omega \to 0$ this becomes identical with the Heller wavepacket for a free particle [15], which is also exact.

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