Shaping and focussing of ionized electron wave packets - Notes on plane-wave wave packets

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(Free wave / plane wave approximation). Investigate ionized electrons in wave packets. Shape and focus. Medium energy, ie. energy is high enough to neglect Coulomb phase contribution allowing us to use plane waves as a good approximation, but at the same time, the energy is low enough to ignore relativistic effects (limit?).

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I. INTRODUCTION

Ionized electrons in wave packets. Shape and focus. Low and medium energy. Combine results from ‘notes-free-wave.tex’ (the free/plane wave approximation for medium energies), with ‘notes-coulomb-func.tex’ (coulomb waves at low energy), and ‘notes-wp-spectrum.tex’ (which looks at the effect of the absorption spectrum on the wave packet),

II. FREE-PARTICLE

A. Time-dependent Schrödinger equation

Time-dependent Schrödinger equation

$$\imath\hbar\frac{\partial\Psi(x,t)}{\partial t} = H\Psi(x,t). \tag{1}$$

For free particle Hamiltonian is

$$H = \frac{p^2}{2m} = \frac{1}{2m}\left(-\imath\hbar\frac{d}{dx}\right)^2 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}. \tag{2}$$

For a time-independent Hamiltonian, we can separate the spatial and time-dependent parts by the ansatz $\Psi(x,t) = \Psi(x)\Psi(t)$. The spatial equation becomes

$$H\Psi(x) = E\Psi(x) \tag{3}$$

which can be rewritten as

$$\left[D_x^2 + k^2\right]\Psi(x) = 0 \tag{4}$$

with $k^2 = 2mE/\hbar^2$. This has the solution

$$\Psi(x) = \frac{1}{\sqrt{2\pi}}e^{\pm\imath kx} \tag{5}$$

where we normalize $\Psi(x)$ so that $\Psi(x) = |k\rangle$, with $\langle k|k'\rangle = \delta(k-k')$. The eigenvalues are

$$E = \frac{\hbar^2k^2}{2m} = \frac{p^2}{2m} \tag{6}$$

where $p = \hbar k$. The time-dependent part is

$$[D_t + \imath\omega]\,\Psi(t) = 0 \tag{7}$$

with $\omega = E/\hbar$ and the solution

$$\Psi(t) = e^{-\imath\omega t}, \tag{8}$$

giving the total solution as

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} e^{\imath kx - \imath\omega t}, \tag{9}$$

where $k \in [-\infty, \infty]$ and $\omega = E/\hbar = \hbar k^2/2m$ according to Equation (6). To summarize, the relation between k, p and ω are

$$\frac{p}{m} = \frac{\hbar k}{m} = \frac{d\omega}{dk}. \tag{10}$$

B. The plane wave solutions

The plane wave solutions $\Psi(x,t)$ have a number of easily established properties. If we fix the position x and vary the time t, and the other way around, we find that

$$T = 2\pi/\omega \tag{11}$$

$$\lambda = 2\pi/k \tag{12}$$

where T is the period of oscillation and λ is the wavelength. Note that $T = 1/\nu$ gives $\omega = 2\pi\nu$ and $E = \hbar\omega = h\nu$.

The *phase velocity* v_p for the plane waves correspond to the motion of points with constant phase (ie. immobile points on the wave). It can simply be obtained by $v_p = \lambda/T = \omega/k$, or directly from the phase as follows. Since the phase is

$$\phi(x,t) = kx - \omega t, \tag{13}$$

$\phi(x,t) = c_0$ (where c_0 is a constant) leads to $x(t) = c_0/k + \omega t/k = x_0 + v_p t$, with the phase velocity $v_p = \omega/k$ and $x_0 = c_0/k$. The phase velocity is half of the classical velocity v_{cl}, since $v_p = \omega/k = p/2m = v_{cl}/2$.

III. WAVE PACKETS

A. General

A wave packet $\Psi(x,t)$ is a superposition of free particle waves

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int dk\, \mathbf{a}(k) e^{\imath kx - \imath\omega t} = \frac{1}{\sqrt{2\pi}} \int dk\, \mathbf{a}(k,t) e^{\imath kx}, \tag{14}$$

where we assume that $a(k,t) = a(k)\exp(-\imath\omega t)$. At $t = 0$ we get

$$\Psi(x, t=0) = \frac{1}{\sqrt{2\pi}} \int dk\, \mathbf{a}(k) e^{\imath kx}. \tag{15}$$

The inverse, given by a Fourier transform[1], is

$$\mathbf{a}(k,t) = \frac{1}{\sqrt{2\pi}} \int dx\, \Psi(x,t) e^{-\imath kx}, \tag{16}$$

where we make use of

$$\delta(k-k') = \frac{1}{2\pi}\int dx\ e^{\imath(k-k')}. \tag{17}$$

We can now investigate the normalization of the wave packet

$$\begin{aligned}
N^2(t) &= \int dx\ |\Psi(x,t)|^2 \\
&= \int dx\ \Psi^*(x,t)\Psi(x,t) \\
&= \int dx \left[\frac{1}{\sqrt{2\pi}}\int dk\ \mathbf{a}(k,t)e^{-\imath kx}\right]^* \\
&\qquad\qquad \left[\frac{1}{\sqrt{2\pi}}\int dk'\ \mathbf{a}(k',t)e^{-\imath k'x}\right] \\
&= \int dk\ \mathbf{a}^*(k,t)\mathbf{a}(k,t) \\
&= \int dk\ \mathbf{a}^*(k)\mathbf{a}(k) \\
&= \int dk\ |\mathbf{a}(k)|^2.
\end{aligned} \tag{18}$$

Equation (18) shows us that;

- the norm is time-independent ($N^2(t) = \mathit{constant}$) and hence probability is preserved
- normalization in real space implies normalization in momentum space (and vice versa).

The last point is an example of the Bessel-Parseval theorem.

1. *Comments on the Dirac notation*

Our results so far can be written compactly in the Dirac notation using the identities $1 = \int dk|k\rangle\langle k|$ and $1 = \int dx|x\rangle\langle x|$. For instance, the representation of the wave packet in k is

$$|\Psi\rangle = \int dk\ |k\rangle\langle k|\Psi\rangle = \int dk\ \frac{e^{\imath kx}}{\sqrt{2\pi}}\mathbf{a}(k)e^{-\imath\omega t}, \tag{19}$$

where we have identified $\langle k|\Psi\rangle = \mathbf{a}(k)e^{-\imath\omega t}$. The conservation of probability is equally simple

$$\langle\Psi|\Psi\rangle = \int dx\ \langle\Psi|x\rangle\langle x|\Psi\rangle = \int dk\ \langle\Psi|k\rangle\langle k|\Psi\rangle \tag{20}$$

where $\langle x|\Psi\rangle = \Psi(x)$ and $\langle k|\Psi\rangle = \Psi(k) = \mathbf{a}(k,t)$. We use the fact that $\langle x|k\rangle = (1/\sqrt{2\pi})\exp(\imath kx)$. The differentiation d/dk is independent of integration over x, and can be taken outside the integral. Hence, $\langle\Psi|k\rangle\langle k|\Psi\rangle = \mathbf{a}(k,t)^*\mathbf{a}(k,t) = \mathbf{a}(k)^*\mathbf{a}(k)$.

B. Motion of wave packet $\langle x(t)\rangle$

$$\langle x(t)\rangle = \int dx\ \Psi^*(x,t)x\Psi(x,t) \tag{21}$$

Replace $\Psi(x,t)$ by the k representation given by Equation (14) and represent x in k space (see Section IX B) by

$$\hat{x} = \imath\frac{d}{dk} \tag{22}$$

which gives

$$\begin{aligned}
\langle x(t)\rangle &= \imath \int dk\, \mathbf{a}^*(k) e^{\imath\omega t} \frac{d}{dk}\mathbf{a}(k) e^{-\imath\omega t} \\
&= \imath \int dk\, \mathbf{a}^*(k) \frac{d\mathbf{a}(k)}{dk} + t \int dk\, \frac{d\omega}{dk}\mathbf{a}^*(k)\mathbf{a}(k) \\
&= I_1 + I_2(t)
\end{aligned} \tag{23}$$

We can solve the two integrals I_1 and $I_2(t)$. The time-dependent integral $I_2(t)$ is

$$\begin{aligned}
I_2(t) &= t \int dk\, \frac{d\omega}{dk} |\mathbf{a}(k)|^2 \\
&= t \int dk\, \frac{\hbar k}{m} |\mathbf{a}(k)|^2 \\
&= v_g t,
\end{aligned} \tag{24}$$

where we have used Equation (10) and where v_g is the group velocity,

$$v_g = \frac{\hbar\langle k\rangle}{m} = \frac{\langle p\rangle}{m} = \langle \frac{d\omega}{dk} \rangle. \tag{25}$$

These averages can be represented in a number of ways in both k and x representations, for instance,

$$\begin{aligned}
v_g &= \frac{1}{m} \int dx\, \Psi^*(x,t) \left(-\imath\hbar \frac{d}{dx} \right) \Psi(x,t) \\
&= \frac{1}{m} \int dk\, \mathbf{a}^*(k,t) \hbar k\, \mathbf{a}(k,t) \\
&= \int dk\, \frac{d\omega}{dk} |\mathbf{a}(k)|^2.
\end{aligned} \tag{26}$$

Note that the group velocity v_g is identical to the classical velocity of a particle with momentum $\langle k\rangle$. For a wave packet with a sufficiently peaked momentum distribution, the group velocity can also be obtained from the stationary phase approximation (see section III B 2 below).

The second, time-independent integral I_1 in Equation (23) is $I_1 = \langle x(0)\rangle = \langle x\rangle_0$. To calculate it, it is convenient to separate phase and amplitude of the momentum distribution function $\mathbf{a}(k)$

$$\mathbf{a}(k) = a(k) e^{\imath\phi(k)} \tag{27}$$

the derivative of which is

$$\frac{d\mathbf{a}(k)}{dk} = \frac{da(k)}{dk} e^{\imath\phi(k)} + \imath a(k) \frac{d\phi(k)}{dk} e^{\imath\phi(k)}. \tag{28}$$

We can now write the integral $I_1 = \langle x\rangle_0$ as

$$\begin{aligned}
I_1 = \langle x\rangle_0 &= \imath \int dk\, a(k) \frac{da(k)}{dk} + \imath a(k)^2 \frac{d\phi(k)}{dk} \\
&= \imath \left[\frac{1}{2} a^2(k) \right] - \int dk\, \frac{d\phi(k)}{dk} a^2(k) \\
&= - \int dk\, \frac{d\phi(k)}{dk} a^2(k)
\end{aligned} \tag{29}$$

because $[a^2(k)]_{-\infty}^{\infty} = 0$ for square integrable functions. So, in summary, the position of the wave packet is given by

$$\langle x(t)\rangle = v_g t + \langle x\rangle_0 \tag{30}$$

with $v_g = \hbar\langle k\rangle/m$.

1. Dirac notation

The very first steps of this derivation can be taken quickly in the Dirac notation as follows

$$\langle\Psi|\hat{x}|\Psi\rangle = \int dk\ \langle\Psi|k\rangle\langle k|\hat{x}|\Psi\rangle = \int dk\ \langle\Psi|k\rangle\imath\frac{d}{dk}\langle k|\Psi\rangle, \tag{31}$$

where we used the result

$$\langle k|\hat{x}|\Psi\rangle = \int dx\ \langle k|x\rangle\langle x|\hat{x}|\Psi\rangle = \int dx\ x\langle k|x\rangle\langle x|\Psi\rangle = \imath\frac{d}{dk}\int dx\langle k|x\rangle\langle x|\Psi\rangle = \imath\frac{d}{dk}\langle k|\Psi\rangle = \imath\frac{d}{dk}\Psi(k). \tag{32}$$

2. Stationary phase approximation

Finally, the group velocity v_g can also be obtained by the stationary phase approximation. The wave packet is, as before,

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int dk\ a(k)e^{\imath kx-\imath\omega t} \tag{33}$$

with the phase $\phi = kx - \omega t$. Assume that $a(k)$ is strongly peaked at $k = k_0$. The position of the center of the wave packet will be where the waves close to k_0 are in phase, ie. $d\phi/dk = 0$. Hence,

$$0 = \left.\frac{d\phi}{dk}\right|_{k=k_0} = x - \left.\frac{d\omega}{dk}\right|_{k=k_0} = x - \frac{\hbar k_0}{m}t \tag{34}$$

which gives $x = v_g t$ with $v_g = \hbar k_0/m$. This agrees with the more general result above as long as $\langle k\rangle \approx k_0$.

C. Dispersion $\triangle x(t)$

The dispersion $\triangle x(t)$ gives an indication of the width of the wave packet. It is defined as

$$\triangle x^2(t) = \langle(x - \langle x\rangle)^2\rangle = \langle x^2\rangle - \langle x\rangle^2. \tag{35}$$

We already obtained the expression for $\langle x(t)\rangle$ in Equation (30) above and consequently we have that

$$\langle x\rangle^2 = \frac{\hbar^2\langle k\rangle^2 t^2}{m^2} + \frac{2\hbar\langle k\rangle\langle x\rangle_0 t}{m} + \langle x\rangle_0^2. \tag{36}$$

We now require $\langle x^2(t)\rangle$,

$$\langle x^2\rangle = \int dx\ \Psi^*(x,t)x^2\Psi(x,t). \tag{37}$$

Change to the k representation (use Equation (22) to rewrite x^2). We have

$$\begin{aligned}
\langle x^2\rangle &= \langle\Psi|\hat{x}^2|\Psi\rangle \\
&= \int \langle\Psi|k\rangle\langle k|\hat{x}^2|\Psi\rangle\ dk \\
&= -\int \langle\Psi|k\rangle \frac{d^2}{dk^2}\langle k|\Psi\rangle\ dk \\
&= -\int \mathbf{a}(k)^* e^{\imath\omega t}\frac{d}{dk^2}\mathbf{a}(k)e^{-\imath\omega t}\ dk \\
&= \int \left[-\mathbf{a}^*\ddot{\mathbf{a}} + 2\imath\mathbf{a}^*\dot{\mathbf{a}}t\dot{\omega} + \imath\mathbf{a}^*\mathbf{a}t\ddot{\omega} + \mathbf{a}^*\mathbf{a}t^2\dot{\omega}^2\right]\ dk \\
&= I_1 + I_2 + \frac{\imath t\hbar}{m} + \frac{t^2\hbar^2\langle k^2\rangle}{m^2}, \qquad (38)
\end{aligned}$$

where in the final step we solve the last two terms in the integral and denote the first two by I_1 and I_2. The dots indicate the derivative d/dk and $\omega = \hbar k/2m$, $\dot{\omega} = \hbar k/m$ and $\ddot{\omega} = \hbar/m$. We can immeditely identify I_1 as $\langle x^2\rangle_0$, ie.

$$I_1 = -\int dk\ \mathbf{a}^*\ddot{\mathbf{a}} = \int dk\ \mathbf{a}^*\left(-\frac{d^2}{dk^2}\right)\mathbf{a} = \int dx\ \Psi(x,0)^* x^2\Psi(x,0) = \langle x^2\rangle_0. \qquad (39)$$

In Dirac notation the same thing goes as follows

$$\langle x^2\rangle_0 = \langle\Psi|x^2|\Psi\rangle = \int \Psi^*(x,0)x^2\Psi(x,0)\ dk = \int\langle\Psi|k\rangle\langle k|x^2|\Psi\rangle\ dk = \int\langle\Psi|k\rangle\left(-\frac{d^2}{dk^2}\right)\langle k|\Psi\rangle = -\int \mathbf{a}^*\ddot{\mathbf{a}}\ dk \qquad (40)$$

To proceed further with I_1 and I_2, we set $\mathbf{a} = a\exp(\imath\phi)$, as in Equation (27) before. This substitution gives that

$$\begin{aligned}
\dot{\mathbf{a}} &= \left(\dot{a} + \imath a\dot{\phi}\right)e^{\imath\phi} \\
\ddot{\mathbf{a}} &= \left(\ddot{a} + 2\imath\dot{a}\dot{\phi} + \imath a\ddot{\phi} - a\dot{\phi}^2\right)e^{\imath\phi}.
\end{aligned} \qquad (41)$$

which in turn allows us to rewrite the integral I_1 as

$$I_1 = \langle x^2\rangle_0 = -\int \mathbf{a}^*\ddot{\mathbf{a}}\ dk = -\int dk\ \left[a\ddot{a} + 2\imath a\dot{a}\dot{\phi} + \imath a^2\ddot{\phi} - a^2\dot{\phi}^2\right] = -\int\left[a\ddot{a} - a^2\dot{\phi}^2\right]dk \qquad (42)$$

where the last equality in Equation (42) follows from

$$\int dk\ \left[\ddot{\phi}a^2 + 2\dot{\phi}a\dot{a}\right] = \int dk\ \frac{d}{dk}\dot{\phi}a^2 = \left[\dot{\phi}a^2\right]_{-\infty}^{\infty} = 0, \qquad (43)$$

which is a consequence of the fact that square integrable functions, such as a, vanish as $k \pm \infty$.

The second integral, I_2, becomes

$$I_2 = 2\imath t\int \mathbf{a}^*\dot{\mathbf{a}}\dot{\omega} = 2\imath t\int a\dot{a}\dot{\omega}\ dk + 2\imath t\int \imath\dot{\phi}a^2\dot{\omega} = -\frac{\imath\hbar t}{m} - 2t\int\dot{\phi}a^2\dot{\omega}, \qquad (44)$$

where we have integrated the first term in parts,

$$\int a\dot{a}\dot{\omega}\ dk = \left[\frac{a^2}{2}\dot{\omega}\right]_{-\infty}^{\infty} - \frac{1}{2}\int\ddot{\omega}a^2\ dk = -\frac{\hbar}{2m}. \qquad (45)$$

Inserting into Equation (38) the results for I_1 in Equation (39) and for I_2 in Equation (44) gives

$$\langle x^2\rangle = \frac{\hbar^2\langle k^2\rangle t^2}{m^2} + \langle x^2\rangle_0 - 2t\int\dot{\phi}a^2\frac{d\omega}{dk}\ dk \qquad (46)$$

As a consequence, we see that $\langle x^2\rangle$ are real as required.

According to Equation (35) and by combining the results from Equations (46) and (36), we have that

$$\triangle x^2(t) = \frac{\hbar^2 \triangle k^2 t^2}{m^2} - \frac{2\hbar\langle k\rangle\langle x\rangle_0 t}{m} - \frac{2\hbar t}{m}Q + \triangle x_0^2 \tag{47}$$

with $\triangle k^2 = \langle k^2\rangle - \langle k\rangle^2$ and $\triangle x_0^2 = \langle x^2\rangle_0 - \langle x\rangle_0^2$, and we define Q as

$$Q = \int dk\ k\dot{\phi}a^2. \tag{48}$$

The dispersion minimum occurs when

$$\frac{d\triangle x^2}{dt} = \frac{d\langle x^2\rangle}{dt} - \frac{d\langle x\rangle^2}{dt} = 0. \tag{49}$$

We can write the derivative of Equation (47) as

$$\frac{d\triangle x^2(t)}{dt} = \frac{2\hbar^2\triangle k^2 t}{m^2} - \frac{2\hbar\langle k\rangle\langle x\rangle_0}{m} - \frac{2\hbar Q}{m}. \tag{50}$$

This Equation is linear with an inclination independent of the phase and is zero when the time $t = t_\triangle$ is

$$\begin{aligned} t_\triangle &= \frac{m^2}{2\hbar^2\triangle k^2}\left[\frac{2\hbar\langle k\rangle\langle x\rangle_0}{m} + 2\int dk\ \dot{\phi}a^2\frac{d\omega}{dk}\right] \\ &= \frac{m}{\hbar\triangle k^2}\left[\int dk\ \left(k - \langle k\rangle\right)\dot{\phi}a^2\right], \end{aligned} \tag{51}$$

where the second equality is obtained using Equation (29). An alternative approach is to complete the square in Equation (47), which gives

$$\triangle x^2(t) = \left(\frac{\hbar\triangle k t}{m} - \frac{\langle k\rangle\langle x\rangle_0}{\triangle k} - \frac{Q}{\triangle k}\right)^2 - \left(\frac{\langle k\rangle\langle x\rangle_0}{\triangle k} + \frac{Q}{\triangle k}\right)^2 + \triangle x_0^2. \tag{52}$$

Using the definition of $t_\triangle$ in Equation (51) we can rewrite Equation (52) as

$$\triangle x^2(t) = \left(\frac{\hbar\triangle k t}{m} - \frac{\hbar\triangle k t_\triangle}{m}\right)^2 - \frac{\hbar^2\triangle k^2 t_\triangle^2}{m^2} + \triangle x_0^2. \tag{53}$$

Clearly, the dispersion minimum in the three equivalent Equations (47), (52) and (53) is

$$\min\left(\triangle x^2\right) = \triangle x_0^2 - \frac{\hbar^2\triangle k^2 t_\triangle^2}{m^2} = \triangle x_0^2 - \frac{\hbar}{m}\left[\int dk\ \left(k - \langle k\rangle\right)\dot{\phi}a^2\right]. \tag{54}$$

It is important to note that Equation (54) is a nonlinear function of the phase. As a consequence, although the time $t_\triangle$ for the minimum in dispersion is a linear function of phase, the actual dispersion is not. This means that contributions to the dispersion from different terms in the phase ϕ are not additive.

For what phase is minimum dispersion achieved? According to earlier results, $\triangle x_0^2$ can be rewritten as

$$\triangle x_0^2 = \langle x^2\rangle_0 - \langle x\rangle_0^2 = \int \dot{\phi}^2 a^2 - a\ddot{a}\ dk - \left[\int \dot{\phi}a^2\ dk\right]^2, \tag{55}$$

where Equation (42) gives $\langle x\rangle_0^2$ and Equation (29) gives $\langle x\rangle_0$. In Equation (55) we can idenitify the phase-free term $\langle x^2_{\text{no phase}}\rangle$ by

$$\langle x^2_{\text{no phase}}\rangle = -\int a\ddot{a}\ dk, \tag{56}$$

which leaves

$$\int \dot{\phi}^2 a^2 \, dk - \left[\int \dot{\phi} a^2 \, dk \right]^2 \geq 0, \tag{57}$$

where the inequality follows from $a^2 \geq 0$, $\dot{\phi}^2 \geq 0$ and $\dot{\phi}^2 \geq \dot{\phi}$. Clearly equality occurs for $\dot{\phi} = 0$, but I am not sure how to show thqt the expression cannot be zero for any other phase ϕ. A proof exists (see eg. Rick Trebino's book and reference to Leon Cohen's work therein).

In this context it is interesting to evaluate the uncertainy relation

$$\triangle k \triangle x \geq \frac{1}{2}, \tag{58}$$

which is the k-form of the uncertainty relation $\triangle p \triangle x \geq \hbar/2$, since $p = \hbar k$. The variation of k is

$$\triangle k^2 = \langle k^2 \rangle - \langle k \rangle^2 \tag{59}$$

with

$$\langle k \rangle = \int \mathbf{a}^* k \mathbf{a} \, dk = \int k a^2 \, dk \tag{60}$$

$$\langle k^2 \rangle = \int \mathbf{a}^* k^2 \mathbf{a} \, dk = \int k^2 a^2 \, dk \tag{61}$$

and clearly $\triangle k$ is independent of the phase and depends on the envelope $a(k)$ only. I have, so far, not been able to derive any general form of the product $\triangle k \triangle x$ which would give interesting physical insight.

For a given momentum distribution $a(k)$, which defines $\triangle k$, it is clear that the dispersion minimum has a lower bound given by the uncertainty principle in Equation (58),

$$\triangle x \geq \frac{1}{2\triangle k}, \tag{62}$$

with equality achieved for instance for a Gaussian $a(k)$ with no phase, $\dot{\phi} = 0$ (see Section III C 1 below). In Section (V) we find the same to be true for a Gaussian with a second-order polynomial phase. *Will all Gaussian pulses achieve the minimum width at some point, irrespective of the phase??* It is possible that equality can be achieved with the phase non-zero, but I am not sure how to investigate this analytically. Clearly one can optimize the phase numerically in order to achieve minimum dispersion. The optimization could be done upon the condition that $t_\triangle$ has a specific value - this is a linear constraint.

We proceed to investigate some special cases.

1. Special cases

A constant phase (ie. $\dot{\phi} \equiv 0$) leads to $Q = 0$ and $\langle x \rangle_0 = 0$ and hence Equation (47) takes the form

$$\triangle x^2 = \frac{\hbar^2 \triangle k^2 t^2}{m^2} + \triangle x_0^2, \tag{63}$$

where we see that for constant phase the minimum dispersion (width) occurs at time $t_\triangle = 0$ and is $\triangle x_0^2$. In this case the wavepacket is $\mathbf{a}(k) = a(k)$ and $\min(\triangle x^2)$ is

$$\min(\triangle x^2) = -\int a\ddot{a} \, dk = \langle x^2 \rangle. \tag{64}$$

For a Gaussian pulse with no phase, we have that at $t = 0$

$$|\Psi\rangle = \frac{1}{2\pi} \int a(k) e^{\imath kx - \imath \omega t} \, dk = \{\text{Assume } t = 0\} = \frac{\epsilon_0}{a} e^{-x^2/2a^2 + ik_0 x}, \tag{65}$$

where $\epsilon_0 = a/\sqrt{\pi}$ and

$$a(k) = \epsilon_0 e^{-\frac{a^2}{2}(k-k_0)^2}. \tag{66}$$

The wave packet is normalized so that $\langle\Psi|\Psi\rangle = 1$. We have that

$$\begin{aligned} \langle k\rangle &= \langle a|k|a\rangle = k_0 & (67)\\ \langle k^2\rangle &= \langle a|k^2|a\rangle = \frac{1}{2a^2} + k_0^2 & (68)\end{aligned}$$

and hence

$$\triangle k^2 = \langle k^2\rangle - \langle k\rangle^2 = \frac{1}{2a^2}. \tag{69}$$

Similarly

$$\begin{aligned} \langle x\rangle &= \langle\Psi|x|\Psi\rangle = 0 & (70)\\ \langle x^2\rangle &= \langle\Psi|x^2|\Psi\rangle = \frac{a^2}{2} & (71)\end{aligned}$$

and so $\triangle x^2 = \langle x^2\rangle - \langle x\rangle^2 = a^2/2$. Hence

$$\triangle k \triangle x = \frac{a}{\sqrt{2}}\frac{1}{\sqrt{2}a} = \frac{1}{2}, \tag{72}$$

and we that at $t = 0$ the Gaussian wave packet is at the Heisenberg uncertainty limit.

IV. POSITION AND DISPERSION

A. Summary of results for arbitrary wave packets

The position of a wave packet is given by Equation (30)

$$\langle x\rangle = v_g t + \langle x\rangle_0, \tag{73}$$

with $v_g = \hbar\langle k\rangle/m$ (from Equation (26)) and

$$\langle x\rangle_0 = -\int dk\, \dot{\phi} a^2, \tag{74}$$

following Equation (29). The wave packet is at the origin when $\langle x(t_{x=0})\rangle = 0$, which means that, by Equation (73),

$$t_{x=0} = -\langle x\rangle_0/v_g. \tag{75}$$

The minimum dispersion, $\min(\triangle x)$, occurs at time $t_\triangle$ (given by Equation (51))

$$t_\triangle = \frac{m}{\hbar\triangle k^2}\int dk\,(k - \langle k\rangle)\dot{\phi} a^2 \tag{76}$$

and the position of the wave packet at time $t = t_\triangle$ is

$$\langle x\rangle_{t_\triangle} = v_g t_\triangle + \langle x\rangle_0 = \frac{\langle k\rangle}{\triangle k^2}\int dk \left(k - \langle k\rangle - \frac{\triangle k^2}{\langle k\rangle}\right)\dot{\phi} a^2. \tag{77}$$

B. Results for polynomial phase

We examine the effect of the phase $\phi(k)$ on the position and dispersion of a wave packet when the phase is given by a general polynomial

$$\phi(k) = \sum_{n=0} \phi_n(k) = \sum_{n=0} c_n k^n, \tag{78}$$

where $n \geq 0$, $n \in$ Integers and $\phi_n(k) = c_n k^n$. Each term in Equation (78) makes a separate, additive, contribution to $\langle x\rangle_0$, $t_{x=0}$, $\langle x\rangle_\triangle$ and $t_\triangle$. This can be seen as follows.

According to Equation (30)), the motion of the center of the wave packet is linear and, according to Equation (26), v_g is independent of phase. The contribution from each term in $\phi(k)$ to $\langle x\rangle_0$ and $t_\triangle$ (and by the linearity of Equation (30) to $\langle x\rangle_\triangle$ and $t_{x=0}$ too) are *additive*.

This can be seen from Equation (29) for $\langle x\rangle_0$, and likewise from Equation (51) for $t_\triangle$. Hence we can evaluate the effect of each phase term in Equation (78) above independently and add the results.

For each term $\phi_n(k) = c_n k^n$ we have that $\dot{\phi}_n = n c_n k^{n-1}$. This gives

$$\begin{aligned}
\langle x\rangle &= v_g t + \langle x\rangle_0 = (\hbar\langle k\rangle/m)t + \langle x\rangle_0 && (79)\\
\langle x\rangle_0 &= -n c_n \langle k^{n-1}\rangle && (80)\\
t_\triangle &= \left(n c_n m/\hbar\triangle k^2\right)\left[\langle k^n\rangle - \langle k\rangle\langle k^{n-1}\rangle\right] = \left(n c_n/v_g\triangle k^2\right)\left[\langle k^n\rangle\langle k\rangle - \langle k\rangle^2\langle k^{n-1}\rangle\right] && (81)\\
\langle x\rangle_\triangle &= v_g t_\triangle + \langle x\rangle_0 = \left(n c_n/\triangle k^2\right)\left[\langle k^n\rangle\langle k\rangle - \langle k^{n-1}\rangle\langle k^2\rangle\right] && (82)\\
t_{x=0} &= -\langle x\rangle_0/v_g = n c_n m\langle k^{n-1}\rangle/\hbar\langle k\rangle && (83)
\end{aligned}$$

For the constant term $n = 0$, $\phi_0(k) = c_0$ and $\dot{\phi} = 0$ gives $\langle x\rangle_{t=0} = \langle x\rangle_\triangle = t_{x=0} = t_\triangle = 0$. Note that at this stage we have made no assumption about the actual *shape* of the distribution $\mathbf{a}(k)$.

For a particular phase $\phi(k)$, given by Equation (78), the different contributions add up as

$$\begin{aligned}
\langle x\rangle &= v_g t + \langle x\rangle_0 && (84)\\
\langle x\rangle_0 &= -\sum_{n\geq 1} n c_n\langle k^{n-1}\rangle && (85)\\
t_\triangle &= \left(m/\hbar\triangle k^2\right)\sum_{n\geq 1} n c_n\left[\langle k^n\rangle - \langle k\rangle\langle k^{n-1}\rangle\right] && (86)\\
\langle x\rangle_\triangle &= v_g t_\triangle + \langle x\rangle_0 && (87)\\
t_{x=0} &= -\langle x\rangle_0/v_g && (88)
\end{aligned}$$

Can we optimize the coefficients c_n in order to achieve: minimum dispersion or a particular position $\langle x\rangle_\triangle$? The position of the dispersion minimum and the corresponding time $t_\triangle$ is a linear function of the coefficients c_n so must be easy to find. The actual dispersion is a nonlinear function of the phase $\phi(k)$ and so requires numerical optimization, possibly with the condition that $t_\triangle$ has a particular value. The dispersion is bounded by the uncertainty principle, where $\triangle k$ depends on the shape of the envelope $a(k)$ only and $\triangle x \geq 1/2\triangle k$, see Equation (62).

V. ANALYTIC WAVE PACKETS

A. Gaussian wave packets with linear and quadratic poynomial phase

1. Introduction

Wave packets for Gaussian distributions $\mathbf{a}(k)$ with phase polynomials of second order or less have analytic expressions given by the Fourier transform of a Gaussian distribution from Section (IX C). A wave packet $\Psi(x,t)$ is a superposition of free particle waves

$$|\Psi(x,t)\rangle = \frac{1}{\sqrt{2\pi}}\int dk\, \mathbf{a}(k) e^{\imath kx - \imath\omega t} \tag{89}$$

with $\omega = \hbar k^2/2m$. The integral in Equation (89) can be viewed as a forward Fourier transform of $\mathbf{a}(k)e^{-\imath\omega t}$ and has an analytic solution when $\mathbf{a}(k)$ is given by

$$\mathbf{a}(k) = a_0 e^{-a^2(k-k_0)^2+\imath\phi(k)} \tag{90}$$

where a_0 is real and the phase function $\phi(k)$ is

$$\phi(k) = p_0 + p_1(k-k_0) + p_2(k-k_0)^2. \tag{91}$$

The analytic solution is given by

$$|\Psi(x,t)\rangle = \tilde{a}_0 e^{-\tilde{a}^2(x+p_1-v_g t)^2+\imath\tilde{\phi}}, \tag{92}$$

where $v_g = \hbar k_0/m$ and

$$\tilde{a}^2 = \frac{1}{4a^2+q^2}, \tag{93}$$

where

$$q = (v_g t - 2p_2 k_0)/ak_0 = [(\hbar t/m) - 2p_2]/a \tag{94}$$

and

$$\tilde{\phi} = p_0 + p_1 k_0 + p_2 k_0^2 + \left(\tilde{a}^2 k_0/2\right)\left[4a^2(2(p_1 - p_2 k_0 + x) - v_g t) + (q/ak_0)(p_1 - 2p_2 k_0 + x)^2\right] \tag{95}$$

and

$$\tilde{a}_0 = a_0\left(de^{\imath\alpha}\right)^{-1/2} \tag{96}$$

with

$$d^2 = 4a^4 + a^2 q^2 \tag{97}$$

and

$$\alpha = \arctan\left(\frac{q}{2a}\right) \tag{98}$$

From Equation (92), and the real part of the exponent in particular, we see that the center of the wave packet moves as

$$x(t) = v_g t - p_1. \tag{99}$$

We also see that the width (dispersion) of the wave packet must be minimum when $\tilde{a}^2$, given by Equation (93), is at its maximum. This occurs when q has its smallest value, ie. when $t = t_\triangle$ is

$$t_\triangle = 2p_2 k_0/v_g = 2p_2 m/\hbar. \tag{100}$$

Finally, the prefactor $\tilde{a}_0$ for the wave packet, given by Equation (96), ensures that when the wave packet changes width (disperses) it remains normalized. We know this to be true in general, ie. for any wave packet, due to the Bessel-Parseval theorem. A closer look at Equation (94) reveals that the dispersion will grow with the square of the time and that more narrow wave packets (a greater) will disperse more slowly.

2. *Normalization*

We know from the Bessel-Parseval theorem that the wave packet will be normalized both in position and in momentum space. We will now confirm this for the analytical formulas obtained for the Gaussian wave packet. First, determine a_0 such that $\langle\Psi|\Psi\rangle = 1$,

$$\langle\Psi|\Psi\rangle = \int \mathbf{a}^*(k)\mathbf{a}(k)\, dk = a_0^2 \int e^{-2a^2(k-k_0)^2}\, dk = a_0^2 \frac{\sqrt{\pi}}{\sqrt{2}a} = 1, \tag{101}$$

which gives $a_0^2 = a\sqrt{2/\pi}$. The corresponding expression in coordinate space is

$$\langle\Psi|\Psi\rangle = |\tilde{a}_0|^2 \int e^{-2\tilde{a}^2(x-(v_g t-p_1))^2}\, dx = |\tilde{a}_0|^2 \frac{\sqrt{\pi}}{\sqrt{2}\tilde{a}} = a_0^2\sqrt{\frac{\pi}{2}}a^{-1} = 1, \tag{102}$$

when $a_0^2 = a\sqrt{2/\pi}$, as expected.

3. *Analytical expressions for dispersion and uncertainty*

Assume a normalized wave packet as above. The $\langle k\rangle$ and $\langle k^2\rangle$ are straightforward to calculate in the k representation,

$$\begin{aligned}\langle k\rangle &= a_0^2 \int k e^{-2a^2(k-k_0)^2}\, dk = k_0 &(103)\\ \langle k^2\rangle &= a_0^2 \int k^2 e^{-2a^2(k-k_0)^2}\, dk = \frac{1}{4a^2} + k_0^2 &(104)\end{aligned}$$

which gives

$$\triangle k^2 = \langle k^2\rangle - \langle k\rangle^2 = \frac{1}{4a^2} \tag{105}$$

and $\triangle k = 1/2a$. We can as easily obtain $\langle x\rangle$ and $\langle x^2\rangle$ in coordinate space,

$$\begin{aligned}\langle x\rangle &= |\tilde{a}_0|^2 \int x e^{-2\tilde{a}^2(x-(v_g t-p_1))^2}\, dx = v_g t - p_1 &(106)\\ \langle x^2\rangle &= |\tilde{a}_0|^2 \int x^2 e^{-2\tilde{a}^2(x-(v_g t-p_1))^2}\, dx = \frac{1}{4\tilde{a}^2} + (v_g t - p_1)^2, &(107)\\ & &(108)\end{aligned}$$

which gives

$$\triangle x^2 = \langle x^2\rangle - \langle x\rangle^2 = a^2 + \frac{(v_g t - 2k_0 p_2)^2}{4a^2 k_0^2}. \tag{109}$$

We see immediately that

$$\min \triangle x^2 = a^2 \tag{110}$$

and that

$$t_\triangle = 2p_2 m/\hbar, \tag{111}$$

in agreement with other derivations.

The uncertainty relation for the analytic Gaussian wave packet thus becomes

$$\triangle x \triangle k = \frac{1}{2}\sqrt{1 + \left[\frac{v_g t - 2k_0 p_2}{2a^2 k_0}\right]^2} = \frac{1}{2}\sqrt{1 + \left[\frac{(\hbar t/2m) - p_2}{a^2}\right]^2} \geq \frac{1}{2}. \tag{112}$$

We see that the wave packet fullfills the Heisenberg uncertainty relation and that its velocity of spreading is proportional to its width in k space. We also see that at time $t_\triangle$ it achieves the minimum width possible, ie. $\triangle x = 1/(2\triangle k)$.

4. Comparison to results for wave packets of arbitrary shape

Lets confirm that the Equation (92) gives results consistent with the general relations in Equations (84) derived earlier for a wave packet of any shape. We expand the phase polynomial

$$\phi(k) = p_0 + p_1(k-k_0) + p_2(k-k_0)^2 = \underbrace{p_0 - p_1 k_0 + p_2 k_0^2}_{c_0} + \underbrace{(p_1 - 2k_0 p_2)}_{c_1} k + \underbrace{p_2}_{c_2} k^2. \tag{113}$$

Inserting this into Equations (84) we obtain

$$\begin{aligned}
\langle x \rangle &= v_g t + \langle x \rangle_0 && (114)\\
\langle x \rangle_0 &= -p_1 && (115)\\
t_\triangle &= 2p_2 m/\hbar && (116)\\
\langle x \rangle_\triangle &= 2p_2 k_0 - p_1 && (117)\\
t_{x=0} &= p_1/v_g && (118)
\end{aligned}$$

where we used $1 = \langle k^0 \rangle$, $k_0 = \langle k \rangle$ and $\triangle k = \langle k^2 \rangle - \langle k \rangle^2$. As expected, these results agree with those for the analytic Gaussian wave packet.

Is there a good way to check the imaginary exponent (phase) in Equation (92)? Compare to numerical results. Would also be fun to use analytic wave packet to look at interference between two identical Gaussian wave packets launched at different times (and again compare to numerical results).

B. Gaussian wave packets with polynomial phase of any order

No analytic solution exists for wave packet with higher order phase polynomials, *but* minimum dispersion $t_\triangle$ and initial position $\langle x \rangle_0$ can be calculated using previous formulas and analytic formulas for higher moments of the Gaussian function (known from statistics). The Gaussian moments are given analytically in Section (IX D).

Let the phase function be

$$\phi(k) = \sum_n c_n (k-k_0)^n \tag{119}$$

such that its derivative is

$$\phi(k) = \sum_n n c_n (k-k_0)^{n-1}. \tag{120}$$

The initial position $\langle x \rangle_0$ is given by Equation (29), which translates into

$$\langle x \rangle_0 = -\sum_n n c_n \langle (k-k_0)^{n-1} \rangle. \tag{121}$$

According to the analytic expressions in Section (IX D), only even n will contribute to this sum. The minimum dispersion $t_\triangle$ is given by Equation (51), and translates into

$$t_\triangle = \frac{m}{\hbar \triangle k^2} \sum_n n c_n \langle (k-k_0)^n \rangle \tag{122}$$

where we used that $\langle k \rangle = k_0$ for a Gaussian distribution. The expressions for $\langle x \rangle_\triangle$ and $t_{x=0}$ follow naturally from these equations. We can rewrite Equations (121) and (122) analytically using the formula for Gaussian moments given by Equation (234). For Equation (122) we then obtain that

$$t_\triangle = \frac{m}{\hbar \triangle k^2} \sum_{n=1} 2n c_{2n} \langle (k-k_0)^{2n} \rangle = \frac{m}{\hbar \triangle k^2} \sum_{n=1} \frac{2n c_{2n} (2n-1)!}{2^{n-1}(n-1)!(2a^2)^n}, \tag{123}$$

where we have exploited the fact that Gaussian moments $\langle (k-k_0)^n \rangle$ are zero for odd n and that their value is known by Equation (234) for n even. Equation (121) in turn becomes

$$\langle x\rangle_0 = -\sum_{n=1}(2n-1)c_{2n-1}\langle (k-k_0)^{2n-2}\rangle = -c_1 - \sum_{n=2}\frac{(2n-1)c_{2n-1}(2n-3)!}{2^{n-2}(n-2)!(2a^2)^{n-1}}. \tag{124}$$

From the two Equation (123) and (124) we see clearly that only even terms in the polynomial c_n will contribute to $t_\triangle$, and only odd terms to $\langle x\rangle_0$. Note that since $\triangle x$ is a non-linear function of the phase, the actual *shape* of the wave function will have a more complicated dependence on the phase.

VI. OPTICAL PULSES

A. Light-matter interaction

First order perturbation theory gives

$$|\Psi(x,t)\rangle = \imath\hbar\int_0^\infty d\omega\; D^-_{ks}(\omega)\mathrm{cef}(\omega,t)|\Psi^-_k(\omega,r)\rangle e^{-\imath\omega t} \tag{125}$$

where for times greater than the duration of the pulse

$$\mathrm{cef}(\omega, t\to\infty) = 2\pi\epsilon(\omega), \tag{126}$$

and the asymptotic wave functions for $r\to\infty$ are

$$|\Psi^-_k(\omega, r\to\infty)\rangle e^{-\imath\omega t} = e^{\imath kr-\imath\omega t}. \tag{127}$$

This last statement needs some qualifying. It is a very good approximation for dissociation wave packets, but in the Coulomb phase there is a non-vanishing Coulomb phase which should strictly speaking be accounted for. We will show, later, that for sufficiently high energies, we can ignore the Coulomb phase to a good approximation.

We have derived most of our results for wave packets for integrals over k. We can rewrite the integral in Equation (125) as an integral over k by

$$\begin{aligned}|\Psi(x,t)\rangle &= \imath\hbar\int_0^{\pm\infty} dk\frac{d\omega}{dk}D^-_{ks}(\omega)\mathrm{cef}(\omega,t)|\Psi^-_k(\omega,r)\rangle e^{-\imath\omega t}\\ &= \frac{\imath\hbar^2}{m}\int_0^{\pm\infty} dk\; kD^-_{ks}(\omega)\mathrm{cef}(\omega,t)|\Psi^-_k(\omega,r)\rangle e^{-\imath\omega t}\end{aligned} \tag{128}$$

where we use $\omega = \hbar k^2/2m$ and $d\omega/dk = \hbar/m$.

While it is natural to discuss optical pulses in terms of their angular frequency $\omega = E/\hbar = 2\pi\nu$, we have so far looked at the wave packets described by distributions in k, $\mathbf{a}(k)$. We will now investigate the effect of optical phase, as given by Equation (131) on the dynamics of wave packets excited in the flat continuum, where the dipole transition moment is approximately constant, $D^-_k(\omega)\approx D^-_k$ over the bandwidth of the optical pulse. In particular, we do not expect the phase to vary much over the width of the pulse. This means that the function $\mathbf{a}(k)$ is given by the optical pulse (except for a complex arbitrary factor D^-_k).

So, to a decent approximation we have that for $t > t_0 + t_{\mathrm{duration}}$

$$|\Psi(x,t)\rangle = 2\pi\frac{\imath\hbar^2}{m}\int_0^{\pm\infty} dk\; kD^-_{ks}\epsilon(\omega)e^{\imath kr-\imath\omega t}$$

where we assume flat continuum and plane waves. Comparison to Equation (14) gives that

$$\mathbf{a}(k) = k\epsilon'(k) \tag{129}$$

where $\epsilon'(k) = \epsilon(\omega)$.

B. Gaussian optical pulse with linear and quadratic phase

A Gaussian pulse can be written in the energy domain as

$$E(\omega) = \epsilon_0 e^{-a^2(\omega-\omega_0)^2+\imath\phi(\omega)} \tag{130}$$

where the phase function $\phi(\omega)$ is

$$\phi(\omega) = p_0 + p_1(\omega-\omega_0) + p_2(\omega-\omega_0)^2 \tag{131}$$

for static, linear and quadratic chirp. The inverse fourier transform is

$$E(t) = \tilde{\epsilon}_0 e^{-\tilde{a}^2(t-p_1)^2+\imath\tilde{\phi}(t)} \tag{132}$$

where

$$\tilde{a}^2 = \frac{a^2}{4(a^4+p_2^2)} \tag{133}$$

and the time-domain phase function $\tilde{\phi}(t)$ is

$$\tilde{\phi}(t) = \alpha + p_0 - \omega_0 t - \frac{p_2(t-p_1)^2}{4(a^4+p_2^2)} \tag{134}$$

with

$$\alpha = \frac{1}{2}\arctan\left(\frac{p_2}{a^2}\right) \tag{135}$$

and

$$\tilde{\epsilon}_0 = \frac{\epsilon_0}{(4a^4+4p_2^2)^{1/4}}. \tag{136}$$

It is important to remember that the expression linear chirp originates in the time domain, from Equation (134) and *not* from Equation (131). The frequency of the oscillation is given by $d\tilde{\phi}(t)/dt$ and for $p_1 = p_2 = 0$ it is constant (ω_0). A linear chirp in $d\tilde{\phi}(t)/dt$ is given by the phase factor p_2, ie. the quadratic term in the energy domain phase given by Equation (131). The phase-shift p_0 does not affect the frequency, nor does the factor p_1, which shifts the time-zero in Equations (132) and (134).

The width (duration) of the pulse is calculated versus the intensity, in particular as a fraction $(1/f)$ of the peak intensity, ie.

$$|E(\omega_0 \pm \delta)|^2 = \frac{\epsilon_0^2}{f} \tag{137}$$

This gives δ as $\delta = \sqrt{\ln f/2a^2}$ and the corresponding width, $\tau = 2\delta$, is

$$\tau_f^\omega = \sqrt{2\ln f/a^2}. \tag{138}$$

In the case of fwhm (full width at half maximum), $f = 2$ and $\tau_{fwhm}^\omega = \sqrt{2\ln 2/a^2}$. In the time domain, the corresponding result is

$$\tau_f^t = \sqrt{2\ln f/\tilde{a}^2}. \tag{139}$$

1. *Wave packet excited with optical linear phase, $\phi(\omega) = p_1(\omega - \omega_0)$ ($\phi(k) \propto ck^2$)*

Assume an optical pulse according to Equation (132), reproduced here for convenience,

$$E(t) = \tilde{\epsilon}_0 e^{-\tilde{a}^2(t-p_1)^2 - \imath\tilde{\phi}(t)}. \tag{140}$$

For $p_0 = p_2 = 0$ we have a linear phase $\phi(\omega) = p_1(\omega - \omega_0)$ which corresponds to a shift in time with the Gaussian pulse envelope centered at time $t = p_1$.

We now convert ω to k using $\omega = \hbar k^2/2m$,

$$p_1(\omega - \omega_0) = \frac{p_1\hbar}{2m}(k^2 - k_0^2) = c(k^2 - k_0^2), \tag{141}$$

where $c = p_1\hbar/2m$. Since this corresponds to $\phi(k) = ck^2$, we obtain from Section (IV B) that

$$\begin{aligned}
\langle x\rangle &= v_g t + \langle x\rangle_0 = v_g(t - p_1) && (142)\\
\langle x\rangle_0 &= -2c\langle k\rangle = -p_1 v_g && (143)\\
t_\triangle &= 2cm/\hbar = p_1 && (144)\\
\langle x\rangle_\triangle &= 0 && (145)\\
t_{x=0} &= 2cm/\hbar = p_1 && (146)
\end{aligned}$$

These relations makes physical sense and are consistent with the optical time shift. For instance, since $t_{x=0} = p_1$ the wave packet appears at $x = 0$ at time $t = p_1$.

2. *Wave packet excited with optica quadratic phase, $\phi(\omega) = p_2(\omega - \omega_0)^2$ ($\phi(k) = ck^4$)*

For $p_0 = p_1 = 0$ we have a quadratic phase $\phi(\omega) = p_2(\omega - \omega_0)^2$, which means that in Equation (132), again reproduced here,

$$E(t) = \tilde{\epsilon}_0 e^{-\tilde{a}^2(t-p_1)^2 - \imath\tilde{\phi}(t)} \tag{147}$$

we get

$$\tilde{a}^2 = \frac{a^2}{4(a^4 + p_2^2)} \tag{148}$$

and

$$\tilde{\phi}(t) = \omega_0 t + \frac{p_2(t)^2}{4(a^4 + p_2^2)} + \alpha/2 \tag{149}$$

with

$$\tan\alpha = p_2/a^2 \tag{150}$$

and

$$\tilde{\epsilon}_0 = \frac{\epsilon_0}{(4a^4 + 4p_2^2)^{1/4}}. \tag{151}$$

From Section (IV B) we have that for $\phi(k) = ck^4$,

$$\begin{aligned}
\langle x \rangle &= v_g t + \langle x \rangle_0 && (152)\\
\langle x \rangle_0 &= -4c\langle k^3 \rangle && (153)\\
t_\triangle &= \frac{4cm}{\hbar \triangle k^2}\left[\langle k^4 \rangle - \langle k \rangle \langle k^3 \rangle\right] && (154)\\
\langle x \rangle_\triangle &= \frac{4c}{\triangle k^2}\left[\langle k^4 \rangle \langle k \rangle - \langle k^3 \rangle \langle k^2 \rangle\right] && (155)\\
t_{x=0} &= 4cm\langle k^3 \rangle / \hbar \langle k \rangle && (156)
\end{aligned}$$

Take a quadratic phase $\phi(\omega) = p_2(\omega - \omega_0)^2$. First, convert to k,

$$p_2(\omega - \omega_0)^2 = c\left(k^4 - 2k_0^2 k^2 + k_0^4\right), \qquad (157)$$

where $c = \frac{p_2 \hbar^2}{4m^2}$. Hence,

$$\phi(k) = ck^4 - 2k_0^2 ck^2 + ck_0^4, \qquad (158)$$

with

$$\dot{\phi}(k) = 4ck^3 + (-2k_0^2)2ck. \qquad (159)$$

This means we have a linear shift in time and a chirp. The different contributions (as a function of k) to $\phi(k)$ are additive, giving

$$\begin{aligned}
\langle x \rangle &= v_g t + \langle x \rangle_0 && (160)\\
\langle x \rangle_0 &= 4c\left[k_0^2 \langle k \rangle - \langle k^3 \rangle\right] && (161)\\
t_\triangle &= \frac{4cm}{\hbar \triangle k^2}\left[\langle k^4 \rangle - \langle k \rangle \langle k^3 \rangle - k_0^2 \triangle k^2\right] && (162)\\
\langle x \rangle_\triangle &= \frac{4c}{\triangle k^2}\left[\langle k^4 \rangle \langle k \rangle - \langle k^3 \rangle \langle k^2 \rangle\right] && (163)\\
t_{x=0} &= -\frac{4cm}{\hbar \langle k \rangle}\left[k_0^2 \langle k \rangle - \langle k^3 \rangle\right] && (164)
\end{aligned}$$

with $c = p_2 \hbar^2 / 4m^2$. We can calculate the moments of k analytically for a Gaussian envelope, using the formulas in Section (IX D). We then find that

$$\begin{aligned}
\langle x \rangle_0 &= -\frac{6ck_0}{a^2} && (165)\\
t_\triangle &= \frac{\hbar p_2}{m}\left[\frac{3}{2a^2} + 2k_0^2\right]. && (166)
\end{aligned}$$

For a narrow pulse, ie. a^2 large, we see that $\langle x \rangle_0 \to 0$ as expected and that $t_\triangle \to 2k_0^2 \hbar p_2 / m$, which means that $t_\triangle$ becomes proportional to p_2 as we would expect.

C. Optical Gaussian pulse with phase linear in k (*unfinished*)

Optical Gaussian pulse with phase linear in k rather than ω, $\phi(k) = ck$. Remains to be written. FT can be found in Renard and Faucher et al (the article contains other interesting phase shapes as well). Examine location and duration ($\langle t \rangle_0$ and $\triangle t^2$) for optical pulse with phase $\phi(\omega) \propto \sqrt{\omega}$. Compare to effect on actual wave packet according to equations below for $\phi(k) = ck$.

$$\begin{aligned}
\langle x \rangle &= v_g t + \langle x \rangle_0 && (167)\\
\langle x \rangle_0 &= -c && (168)\\
t_\triangle &= 0 && (169)\\
\langle x \rangle_\triangle &= -c && (170)\\
t_{x=0} &= cm/\hbar\langle k \rangle && (171)
\end{aligned}$$

Explore pulses with $\phi(k) = ck$, ie. $\sqrt{\omega}$ chirp. Check FT - duration, position? Calculate cef. Investigate effect on position and dispersion of wp.

D. Gaussian pulse with sinusoidal phase (*unfinished*)

Write... Characterize wave packets excited by Gaussian pulse with sinusoidal phase.

E. Defining wave packet in k vs in ω

At some point I was concerned about the differences between defining the envelope of the wave packet in k or in ω. The two following sections investigate two aspects of this. The first one compares the effect of changing k_0 or ω_0 on the wave packet. The second section investigates the changes in the width of the wave packet when changing k_0 vs ω_0.

1. *The effect of changing k_0 vs. changing ω_0*

For a Gaussian distribution $a(k)$ in momentum, centered at k_0, we have that $\langle k \rangle = k_0$. While the velocity of the center of the wave packet, $v_g = \hbar\langle k \rangle = \hbar k_0$, depends on k_0, the shape of the wave packet does not. Hence the dispersion, *as a function of time*, will be the same regardless of the value of k_0. On the other hand, the position of the wave packet, $\langle x \rangle = v_g t + \langle x \rangle_0$, will be different, and consequently the dispersion *as a function of position* $\langle x \rangle$ will be different for different k_0.

The same is not true when the wave packet is defined by e.g. an excitation pulse centered at ω_0 and the value of ω_0 is changed. Because of the non-linear relationship between k and ω, different ω_0 correspond to different momentum distributions. A higher ω_0 will result in a wider spread of momenta, and hence in a broader pulse in the coordinate representation. This can be approximately compensated for by making the pulse with higher ω shorter, as described in the next Section VI E 2.

2. *Width in position x as function of ω_0*

The width of the pulse in the x coordinate, τ_x, is directly linked to the width in momentum space τ_k. A pulse with momentum distribution $\mathbf{a}(k - k_0)$ will have the same width regardless of the actual value of k_0, as long as the shape of the distribution is constant around k_0.

On the other hand, a fixed pulse-shape in the energy domain, $E(\omega)$, will give rise to a different distribution in momentum space (k), depending on the value of ω_0. This is due to the non-linear relationship between k and ω ($\omega = \hbar k^2/2m$).

Assuming a Gaussian optical pulse, the pulse width with regards to the pulse *amplitude* (not intensity) is

$$\tau_\omega = \sqrt{4 \ln f / a^2}. \tag{172}$$

The pulse envelope is a fraction $1/f$ of the peak amplitude when $\omega = \omega_0 \pm \tau_\omega/2$. This corresponds to

$$k_\pm = \sqrt{\frac{2m\,(\omega_0 \pm \tau_\omega/2)}{\hbar^2}} = \frac{\sqrt{2m\omega_0}}{\hbar}\sqrt{1 \pm \tau_\omega/2\omega_0}. \tag{173}$$

When $\tau_\omega \ll \omega_0$, first order Taylor expansion gives

$$k_\pm \approx \frac{\sqrt{2m\omega_0}}{\hbar}\left(1+\frac{\tau_\omega}{4\omega_0}\right). \tag{174}$$

The corresponding width in k is then

$$\tau_k = k_+ - k_- = \tau_\omega\sqrt{\frac{m}{2\hbar^2\omega_0}}. \tag{175}$$

We can now quickly estimate the width in x by taking a wave packet constructed from three plane waves, with momentum k_0 and $k_0 \pm \tau_k/2$, ie.

$$\begin{aligned}\Psi(x) &= e^{\imath k_0 x} + e^{\imath(k_0-\tau_k/2)x} + e^{\imath(k_0+\tau_k/2)x} &(176)\\ &= e^{\imath k_0 x}\left(1+\cos\frac{\tau_k x}{2}\right) &(177)\end{aligned}$$

The wave function $\Psi(x)$ will be zero when $\tau_k x/2 = \pm\pi$ and hence $x = \pm 2\pi\tau_k$. This in turn implies that $\tau_x = 4\pi/\tau_k$. The corresponding Heisenberg uncertainty is

$$(\tau_k)(\tau_x) = 4\pi \tag{178}$$

which is well above the Heiseberg uncertainty limit. Inserting the definition of τ_k and τ_ω into the expression for τ_x gives

$$\tau_x = \frac{4\pi}{\tau_k} = \sqrt{\frac{8\pi^2\hbar^2 a^2\omega_0}{m\ln f}} \tag{179}$$

So, if we change ω_0 and want to keep (approximately) the same width τ_x of the wave packet, we need to make sure that the product $a^2\omega_0$ remains constant. So if the first experiment has $\omega_0^{(1)}$ and $a_1^2\omega_0 = c_0$, then the second experiment at $\omega_0^{(2)}$ requires $a_2^2 = c_0/\omega_0^{(2)}$. The corresponding durations of the two pulses are

$$\begin{aligned}\tau_t^{(1)} &= \sqrt{2\ln f/\tilde{a}_1^2} &(180)\\ \tau_t^{(2)} &= \sqrt{2\ln f/\tilde{a}_2^2}, &(181)\end{aligned}$$

with

$$\tilde{a}_i^2 = \frac{a_i^2}{4(a_i^4+p_2^2)}, \tag{182}$$

and

$$a_i^2\omega_0^{(i)} = c_0. \tag{183}$$

VII. CALCULATIONS

A. Understanding dispersion

In Figure 1 we investigate dispersion. We see that dispersion of the wave packet is a consequence of the non-linear dispersion relation $\omega = \hbar k^2/2m$, and that wave packets propagated with a linear dispersion relation $\omega = k$ do not disperse.

The dispersion relation can be seen as a convolution

$$|\Psi(x,t)\rangle = \int dk\ g(k)e^{-\imath\omega t}e^{\imath kx} = \int dk\ g(k)f(k)e^{\imath kx} = g(k)\otimes f(k), \tag{184}$$

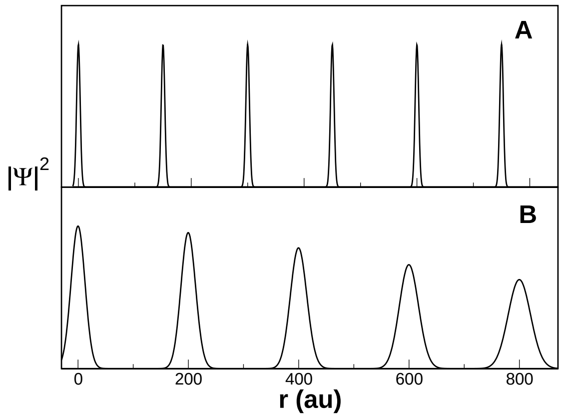


FIG. 1: These two sequences of wave packets illustrate the role of the dispersion relation in dispersion. In both cases, snapshots of the propagating wave packet at different times are shown. The first sequence of wave packets (A) is generated with a (fictional) linear dispersion relation $\omega = k$, while the second (B) is generated with the normal, non-linear dispersion relation $\omega = \hbar k^2/2m$.

where

$$f(k) = e^{-\imath\omega t} \tag{185}$$

with $\omega = \hbar k^2/2m$ and the convolution is

$$f(k) \otimes g(k) = \int d\omega' \; f(\omega')g(\omega - \omega'). \tag{186}$$

The problem is that, as far as I can tell (Mathematica) $f(k)$ does not have a Fourier transform $f(\omega)$.

The big question I would want to answer is: why is $|\Psi(x, t \to \infty)| \propto$ spectrum? In a classical sense the high energy components will move the furthest away and the amount of each component will be proportional to the spectrum.

B. Focussing of wave packets with linear chirp

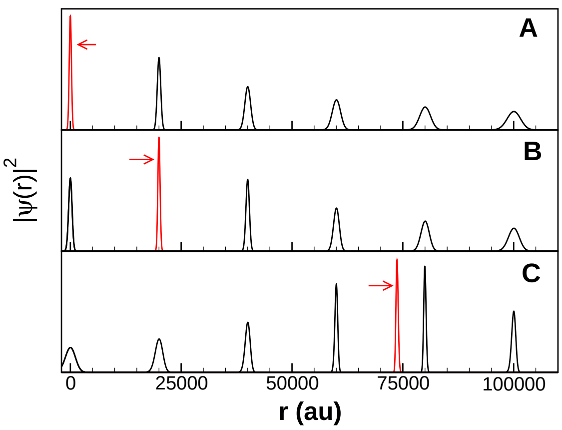


FIG. 2: Wave packet generated by a Gaussian pulse with positive chirp ($p_2 > 0$). (A) No chirp, dispersion increases monotonically as the wave packet propagates, (B) Weak chirp, the wave packet is focussed at $r \approx 20000$ au, and (C) Stronger chirp, the wave packet is focussed at $r \approx 75000$ au.

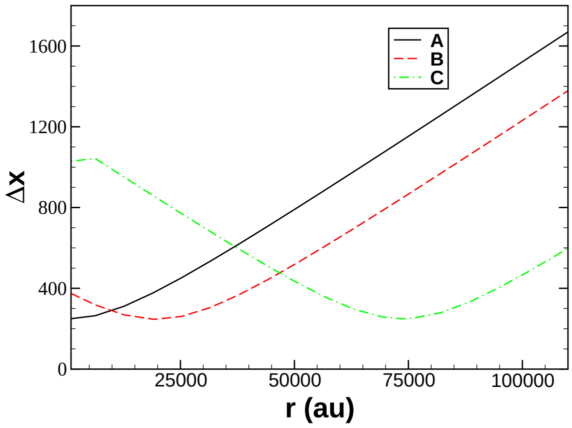


FIG. 3: Dispersion (width), $\triangle x$, as a function of position for wave packets A-C in Figure 2. (A) No chirp, (B) Weak chirp and (C) Stronger chirp

In this Section we investigate the focussing of wave packets with linear chirp in time. This corresponds to a quadratic phase in the energy domain.

- make issue of t_0 for optical pulse clearer. for instance, does $\langle x \rangle_0 \neq 0$ imply that $t_0 \neq 0$ for the corresponding optical pulse??
- work out maths, so that for wave packets with given k_0, one can directly calculate which chirp is required to focus pulse at a particular radial distance. Note that one should include some check that the focus point is further out than $x = v_g \tau_t$, where τ_t is the duration of the pulse at the given chirp.

1. Classical interpretation of linear chirp focussing

A classical, non-mathematical explanation for why a positive chirp is required to focus the wave packet at distances $x > 0$; For positive chirp, higher frequencies (energy) components of the wave packet are excited after the slower components. As the faster components overtake the slow, the wave packet narrows. For negative chirp, the fast components are released first and the wave packet can only broaden.

C. Gaussian wave packet

$$|\Psi(x,t)\rangle = \frac{1}{(2\pi\hbar)^{D/2}} \int g(k) e^{\imath kr - \imath\omega t} dk \tag{187}$$

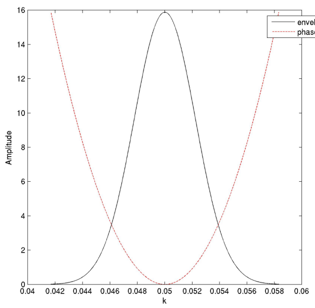
$\omega = \frac{\hbar k^2}{2m} = \frac{E}{\hbar}$. $p = \hbar k$. Assume transform limited Gaussian optical pulse and structureless continuum. $g(k)$ gaussian. $\Psi(x,0) = e6{-}x^2/2a^2$. $g(k) \propto \epsilon(k) = \epsilon_0 e^{-\alpha(k-k_0)^2}$. This integral can be solved analytically

$$\Psi(x,t) = \frac{e^{-\frac{x^2}{2(a^2 + (\imath\hbar/m)t)}}}{\sqrt{1 + (\imath\hbar t/ma^2)}} \tag{188}$$

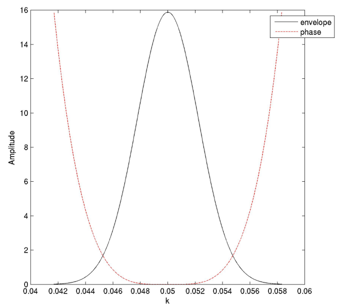
$g(k,t) = FT(\Psi(x,t))$, $|g(k,t)|^2 =$ constant in time.

D. Gaussian wave packets with polynomial phase

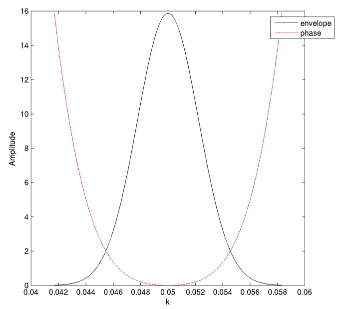
We evaluate numerically Gaussian wave packets in k space with polynomial phase $\phi(k) = \sum c_n(k-k_0)^n$, as disussed in Section (V B).



(a)Phase polynomial 1a



(b)Phase polynomial 1b



(c)Phase polynomial 1c(=1a+1b)

FIG. 4: Gaussian envelope and polynomial phase for wave packet in k space.

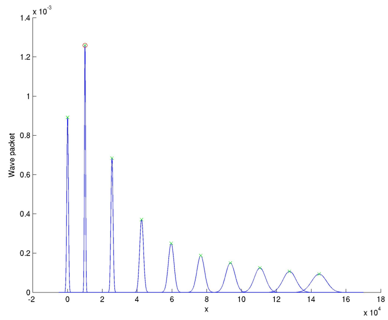
In all cases the reference wave packet is the zero-phase polynomial, $\phi(k) \equiv 0$, ie. $\{c_n\} = \{0,0,0,0\}$. First we investigate three phase polynomials that change $t_\triangle$ but do not alter $\langle x\rangle_0 = 0$. This requires that only even orders are included. The three sets of coefficients are

$$\begin{aligned} &\{c_n\} = \{c_0, c_1, c_2, c_3, c_4\} \\ \text{1a:}\ &\{c_n\} = \{0,0,a^2,0,0\} \quad \text{(2nd order only)} \\ \text{1b:}\ &\{c_n\} = \{0,0,0,0,\frac{2a^4}{3}\} \quad \text{(4th order only)} \\ \text{1c:}\ &\{c_n\} = \{0,0,1a^2,0,\frac{2a^4}{3}\} \quad \text{(2nd and 4th order)} \end{aligned} \tag{189}$$

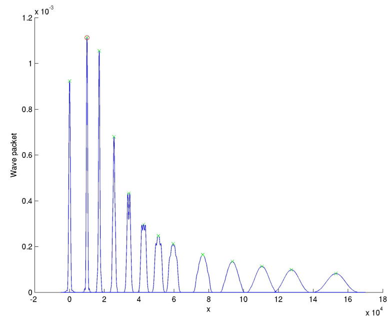
Second, we investigate three phase polynomials that change $\langle x\rangle_0$ only. The three sets of coefficients are

$$\begin{aligned} &\{c_n\} = \{c_0, c_1, c_2, c_3, c_4\} \\ \text{2a:}\ &\{c_n\} = \{0,-2500,0,0,0\} \quad \text{(1st order only)} \\ \text{2b:}\ &\{c_n\} = \{0,0,0,-2500\frac{4a^2}{3},0\} \quad \text{(3rd order only)} \\ \text{2c:}\ &\{c_n\} = \{0,-2500,0,-2500\frac{4a^2}{3},0\} \quad \text{(1st and 3rd order)} \end{aligned} \tag{190}$$

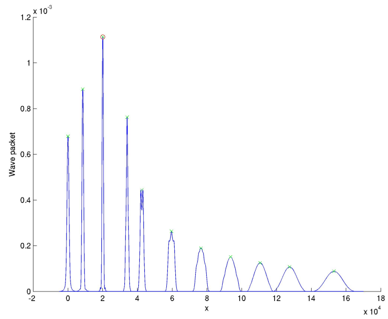
and we see that only odd orders are non-zero in the phase polynomial.



(a)1a, $\langle x \rangle_0 = 0$, $t_{\triangle} = 2 \times 10^5$



(b)1b, $\langle x \rangle_0 = 0$, $t_{\triangle} = 2 \times 10^5$



(c)1c, $\langle x \rangle_0 = 0$, $t_{\triangle} = 4 \times 10^5$

FIG. 5: Numerical wave packet generated by phase polynomials 1a, 1b and 1c. The wave packets are plotted as a function of position at different times, $t \geq 0$. The center of the wave packet, according to the formula $\langle x \rangle = v_g t + \langle x \rangle_0$, is indicated by an 'x' at each time, and the dispersion minimum is indicated with a red circle. Note that $\langle x \rangle_0 = 0$ in all three cases and that v_g is identical for each Gaussian wave packet.

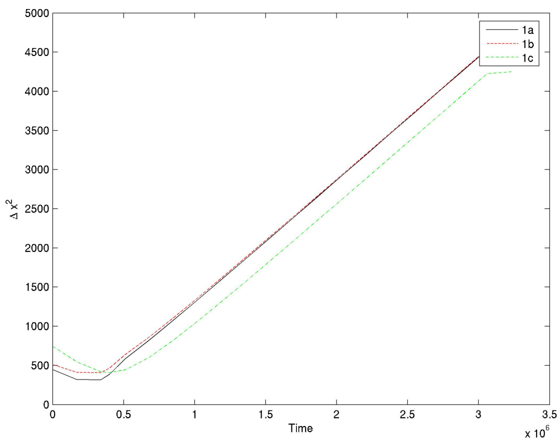
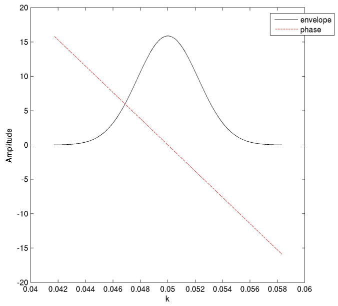


FIG. 6: Dispersion (width), $\triangle x$, as a function of time for wave packets 1a, 1b and 1c. Note that a) the higher order terms increase the minimum, b) the shift in (c) is additive, c) the velocity of spreading (ie the inclination) is identical in all three cases.

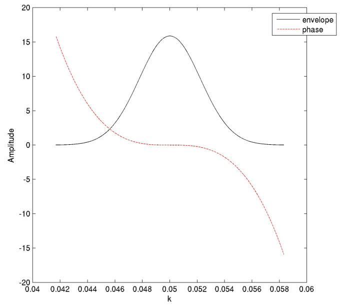
E. Shape of wave packets, from excitation to asymptote

Initially, the excited wave packet mimics the time-domain shape of the excitation pulse. On the other hand, the asymptotic form is proportional to the energy-domain shape. In between, the wave packet is distorted by interference.

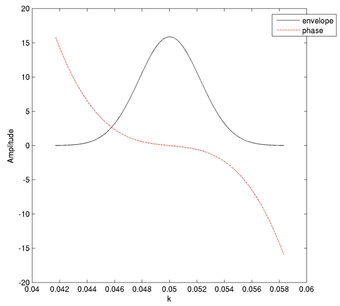
Since the wave packet at large times / distances returns to the energy-domain shape (product of absorption spectrum and pulse), can we do 'spectroscopy' by characterizing wave packet through x-ray scattering? Or can one get immediate



(a)Phase polynomial 2a

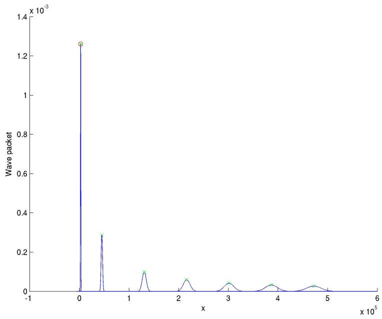


(b)Phase polynomial 2b

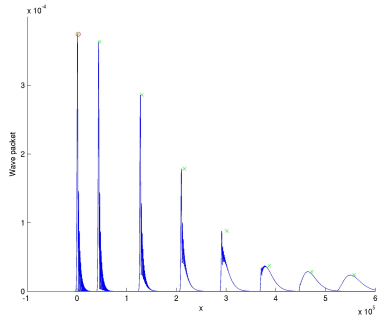


(c)Phase polynomial 2c(=2a+2b)

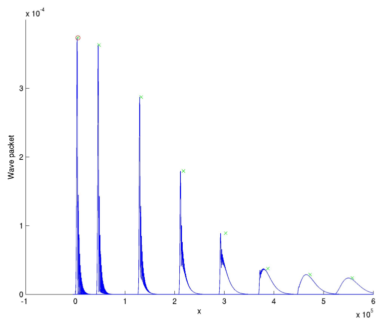
FIG. 7: Gaussian envelope and (polynomial) phase for wave packet in k space.



(a)2a, $\langle x \rangle_0 = 2500$, $t_\triangle = 0$



(b)2b, $\langle x \rangle_0 = 2500$, $t_\triangle = 0$



(c)2c, $\langle x \rangle_0 = 5000$, $t_\triangle = 0$

FIG. 8: Numerical wave packet generated by phase polynomials 2a, 2b and 2c. The wave packets are plotted as a function of position at different times, $t \geq 0$. The center of the wave packet, according to the formula $\langle x \rangle = v_g t + \langle x \rangle_0$, is indicated by an 'x' at each time, and the dispersion minimum is indicated with a red circle. Note that $t_t riangle = 0$ in all three cases and that v_g is identical for each Gaussian wave packet.

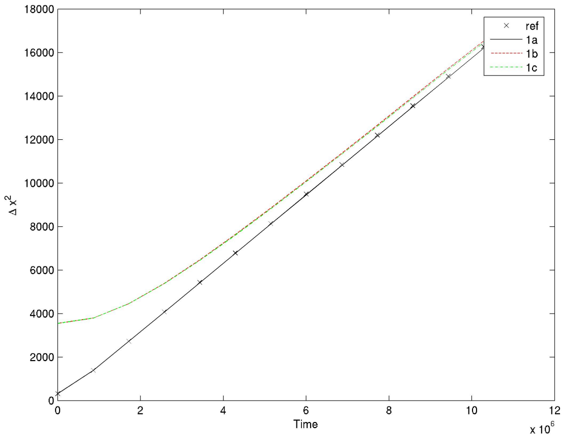


FIG. 9: Dispersion (width), $\triangle x$, as a function of time for wave packets 2a, 2b and 2c and the reference wave packet with no phase. Note that the linear phase term only shifts the initial position of the wave packet, while the dispersion as a function of *time* is identical to the reference wave packet with no phase. The minimum dispersion is greater for the wave packets with higher order terms and the asymptotic velocity of spreading is the same in all four cases.

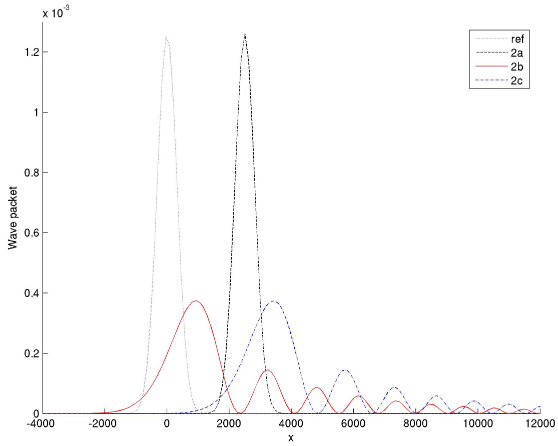


FIG. 10: Wave packets at time $t = 0$ for phase polynomials 2a, 2b, 2c and the reference wave packet (dashed line). Note that the first order term in the polynomial shifts the wave packet *without any distortion*, which can be seen by comparing 2a with the reference wave packet and 2b with 2c. Also note that the wave packets for phases 2a and 2b both have the same $\langle x \rangle_0 = 2500$, yet appear quite different. Wave packet 2b, which has a higher order phase term is quite spread out, with the main 'bump' centered at distances smaller than $\langle x \rangle_0$.

information on the spectrum covered by the ultrashort pulse through the use of an atomic streak camera? Clearly some issues with incredibly low electron density at required distances. Strong field will give more complex, hard to interpret spectra. Focussing wave packet with external fields? Too much distortion? Maybe non-gaseous samples are better - what about photoelectrons from surfaces?

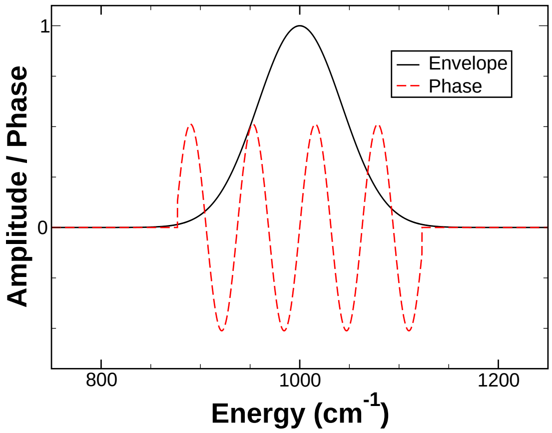


FIG. 11: Phase and envelope for Gaussian pulse with sinusoidal phase. The phase is $\phi(\omega) = \sin(10(\omega - \omega_0)/\tau_\omega)$.

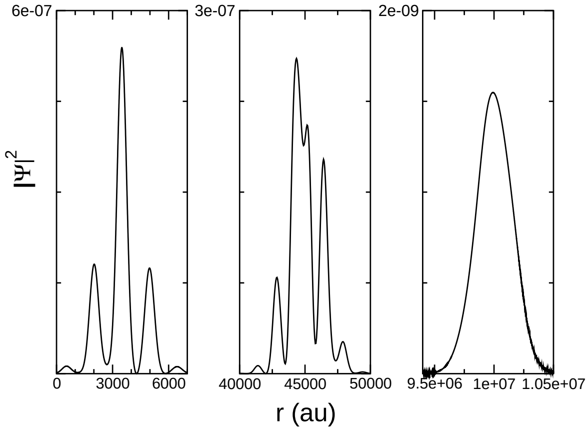


FIG. 12: Wave packet generated by the sinusoidal phase in Figure 11 at three different radial distances r. At small distances, the wave packet mimics the shape of the time-dependent pulse. At intermediate distance it has a distorted shape, and finally, at asymptotic distances it assumes the energy-domain shape (in this case, a Gaussian).

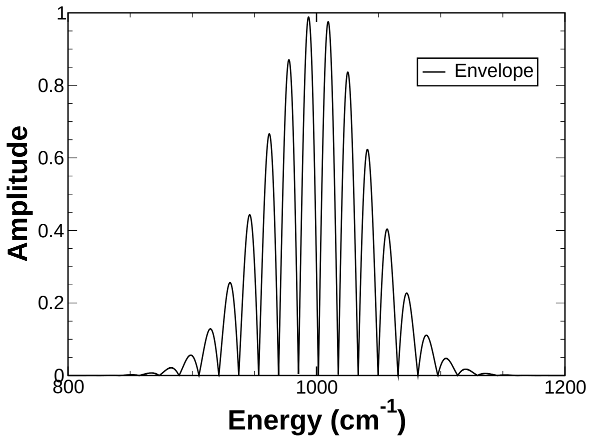


FIG. 13: Phase and envelope for two coherent Gaussian pulses. The Fourier transform of two identical Gaussian pulses, the first centered at time $t = 0$ and the second at $t = \triangle$, is $G(\omega)\cos(\omega\triangle/2)e^{\imath\omega\triangle/2}$, where $G(\omega)$ is a Gaussian envelope. In the present case $\triangle = 10\tau_t$.

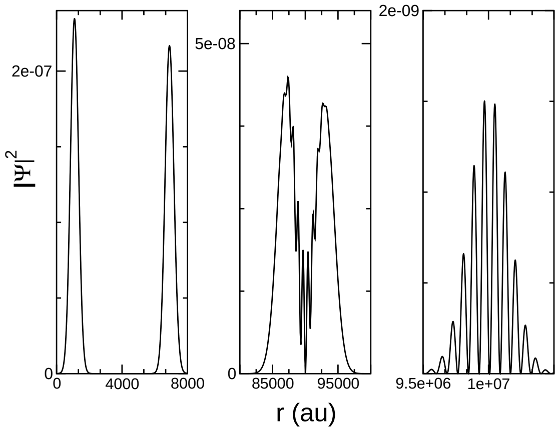


FIG. 14: Wave packet generated by two coherent Gaussian pulses, as shown in Figure 13, at three different radial distances r. At small distances, the wave packet mimics the shape of the time-dependent pulse. At intermediate distance it has a distorted shape due to interference, and finally, at asymptotic distances it assumes the energy-domain shape (in this case, a modulated Gaussian).

VIII. SUMMARY

IX. ADDITIONAL NOTES

A. To do

- 'rewind' idea: choose shape of wp at particular position, propagate back to origin and calculate required pulse, based on absorption spectrum.

B. Coordinate to momentum and back

$$\mathbf{1} = |p\rangle\langle p| \tag{191}$$
$$\mathbf{1} = |r\rangle\langle r| \tag{192}$$

$$\Psi(r) = \int |r\rangle\langle r|\Psi\rangle dr = \int |p\rangle\langle p|r\rangle\langle r|\Psi\rangle dp = \int |p\rangle\langle p|\Psi\rangle dp \tag{193}$$

$$\langle p|r\rangle = e^{\imath pr} \tag{194}$$

$$\langle x'|x''\rangle = \int \delta(x-x')\delta(x-x'')dx = \delta(x'-x'') \tag{195}$$

$$\langle p'|p''\rangle = \int \delta(p-p')\delta(p-p'')dp = \delta(p'-p'') \tag{196}$$

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\imath px/\hbar} \tag{197}$$

Find x and p in the coordinate representation:

$$\langle x|\hat{x}|\Psi\rangle = x\langle x|\Psi\rangle = x\Psi(x) \tag{198}$$

and so $\hat{x} = x$.

$$\langle x|\hat{p}|\Psi\rangle = \int dp\ \langle x|p\rangle\langle p|\hat{p}|\Psi\rangle = \int dp\ p\langle x|p\rangle\langle p|\Psi\rangle = -\imath\hbar\frac{d}{dx}\int dp\ \langle x|p\rangle\langle p|\Psi\rangle = -\imath\hbar\frac{d}{dx}\langle x|\Psi\rangle = -\imath\hbar\frac{d}{dx}\Psi(x) \tag{199}$$

and so $\hat{p} = -\imath\hbar\frac{d}{dx}$.

Find x and p in the momentum representation:

$$\langle p|\hat{p}|\Psi\rangle = p\langle p|\Psi\rangle = p\Psi(p) \tag{200}$$

and so $\hat{p} = p$.

$$\langle p|\hat{x}|\Psi\rangle = \int dx\ \langle p|x\rangle\langle x|\hat{x}|\Psi\rangle = \int dx\ x\langle p|x\rangle\langle x|\Psi\rangle = \imath\hbar\frac{d}{dp}\int dx\ \langle p|x\rangle\langle x|\Psi\rangle = \imath\hbar\frac{d}{dp}\langle p|\Psi\rangle = \imath\hbar\frac{d}{dp}\Psi(p) \tag{201}$$

and so $\hat{x} = \imath\hbar\frac{d}{dp}$.

The k representation is essentially identical to the momentm representation since $\hat{p} = \hbar\hat{k}$.

$$\langle k'|k''\rangle = \delta(k' - k'') \tag{202}$$

$$\langle x|k\rangle = \frac{e^{\imath kx}}{\sqrt{2\pi}} \tag{203}$$

$$\langle k'|k''\rangle = \int dx\ \langle k'|x\rangle\langle x|k''\rangle = \int dx\ \frac{e^{-\imath k'x}}{\sqrt{2\pi}}\frac{e^{\imath k''x}}{\sqrt{2\pi}} = \frac{1}{2\pi}\int dx\ e^{\imath(k'-k'')x} = \delta(k'' - k') \tag{204}$$

C. Fourier transform of Gaussian

We define the Fourier transform as

$$f(t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(\omega)e^{\imath\omega t}\ d\omega \tag{205}$$

and the inverse Fourier transform as

$$f(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(t)e^{-\imath\omega t}\ dt. \tag{206}$$

Note that changing $t \to -t$ in Equation (205) amounts to

$$f(-t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(\omega)e^{-\imath\omega t}\ d\omega, \tag{207}$$

ie. a trivial difference. Often in modern physics the 2π factor enters asymmetrically, with the full factor $1/2\pi$ entering in the inverse transform.

A Gaussian (normal) distribution with a phase $\phi(\omega)$ can be written

$$E(\omega) = \epsilon_0 e^{-a^2(\omega-\omega_0)^2+\imath\phi(\omega)} \tag{208}$$

where the phase function $\phi(\omega)$ is

$$\phi(\omega) = p_0 + p_1(\omega - \omega_0) + p_2(\omega - \omega_0)^2. \tag{209}$$

The inverse Fourier transform is

$$E(t) = \tilde{\epsilon}_0 e^{\imath\alpha} e^{-\imath\frac{(t-p_1)^2}{4(p_2+\imath a^2)}+\imath p_0-\imath\omega_0 t} \tag{210}$$

with

$$\alpha = \frac{1}{2}\arctan\left(\frac{p_2}{a^2}\right) \tag{211}$$

and

$$\tilde{\epsilon}_0 = \frac{\epsilon_0}{(4a^4+4p_2^2)^{1/4}}. \tag{212}$$

The exponent in Equation (210) can be rewritten in a form more similar to Equation (208),

$$E(t) = \tilde{\epsilon}_0 e^{-\tilde{a}^2(t-p_1)^2+\imath\tilde{\phi}(t)} \tag{213}$$

by

$$\tilde{a}^2 = \frac{a^2}{4(a^4+p_2^2)} \tag{214}$$

and the time-domain phase function $\tilde{\phi}(t)$

$$\tilde{\phi}(t) = \alpha + p_0 - \omega_0 t - \frac{p_2(t-p_1)^2}{4(a^4+p_2^2)} \tag{215}$$

with α and $\tilde{\epsilon}_0$ defined as in Equations (211-212).

The inverse Fourier transform of

$$f(\omega) = \epsilon_0 e^{-a^2(\omega-\omega_0)^2+\imath(p_0+p_1\omega+p_2\omega^2)} \tag{216}$$

is

$$f(t) = \tilde{\epsilon}_0 e^{\imath p_0 - a^2\omega_0^2 - \imath\frac{(t-p_1+2\imath a^2\omega_0)^2}{4(p_2+\imath a^2)}} \tag{217}$$

with

$$\tilde{\epsilon}_0 = \epsilon_0/\sqrt{2}\sqrt{a^2-\imath p_2} \tag{218}$$

D. Moments of the Gaussian distribution

We find it useful to have the moments $\langle k^n\rangle$ of the Gaussian (normal) distribution,

$$\langle k^n\rangle = \int_{-\infty}^{\infty} k^n e^{-a^2(k-k_0)^2}\, dk, \tag{219}$$

which we obtain from *Mathematica* for orders $n = 0-7$. $n = 0$

$$\frac{\sqrt{\pi}}{a} = \int_{-\infty}^{\infty} e^{-a^2(k-k_0)^2}\, dk, \tag{220}$$

$n = 1$

$$k_0\frac{\sqrt{\pi}}{a} = \int_{-\infty}^{\infty} k e^{-a^2(k-k_0)^2}\, dk, \tag{221}$$

$n = 2$

$$\frac{(1 + 2a^2k_0^2)}{2a^2}\frac{\sqrt{\pi}}{a} = \int_{-\infty}^{\infty} k^2 e^{-a^2(k-k_0)^2}\ dk, \tag{222}$$

$n = 3$

$$\frac{k_0(3 + 2a^2k_0^2)}{2a^2}\frac{\sqrt{\pi}}{a} = \int_{-\infty}^{\infty} k^3 e^{-a^2(k-k_0)^2}\ dk, \tag{223}$$

$n = 4$

$$\frac{(3 + 12a^2k_0^2 + 4a^4k_0^4)}{4a^4}\frac{\sqrt{\pi}}{a} = \int_{-\infty}^{\infty} k^4 e^{-a^2(k-k_0)^2}\ dk, \tag{224}$$

$n = 5$

$$\frac{k_0(15 + 20a^2k_0^2 + 4a^4k_0^4)}{4a^4}\frac{\sqrt{\pi}}{a} = \int_{-\infty}^{\infty} k^5 e^{-a^2(k-k_0)^2}\ dk, \tag{225}$$

$n = 6$

$$\frac{(15 + 90a^2k_0^2 + 60a^4k_0^4 + 8a^6k_0^6)}{8a^6}\frac{\sqrt{\pi}}{a} = \int_{-\infty}^{\infty} k^6 e^{-a^2(k-k_0)^2}\ dk, \tag{226}$$

$n = 7$

$$\frac{k_0(105 + 210a^2k_0^2 + 84a^4k_0^4 + 8a^6k_0^6)}{8a^6}\frac{\sqrt{\pi}}{a} = \int_{-\infty}^{\infty} k^7 e^{-a^2(k-k_0)^2}\ dk, \tag{227}$$

It is also helpful, especially when evaluating phase functions, to have the moments for $\langle (k-k_0)^n \rangle$ for the Gaussian distribution,

$$\langle (k-k_0)^n \rangle = \int_{-\infty}^{\infty} (k-k_0)^n e^{-a^2(k-k_0)^2}\ dk, \tag{228}$$

which we obtain from *Mathematica* for orders $n = 1 - 7$. Since the Gaussian distribution is an even function around k_0, the integral will be zero for $n \in$ Odd.

For the first five even orders we have that, $n = 2$

$$\frac{1}{2a^2}\frac{\sqrt{\pi}}{a} = \int_{-\infty}^{\infty} (k-k_0)^2 e^{-a^2(k-k_0)^2}\ dk, \tag{229}$$

$n = 4$

$$\frac{3}{4a^4}\frac{\sqrt{\pi}}{a} = \int_{-\infty}^{\infty} (k-k_0)^4 e^{-a^2(k-k_0)^2}\ dk, \tag{230}$$

$n = 6$

$$\frac{15}{8a^6}\frac{\sqrt{\pi}}{a} = \int_{-\infty}^{\infty} (k-k_0)^6 e^{-a^2(k-k_0)^2}\ dk, \tag{231}$$

$n = 8$

$$\frac{105}{16a^8}\frac{\sqrt{\pi}}{a} = \int_{-\infty}^{\infty} (k-k_0)^8 e^{-a^2(k-k_0)^2}\ dk, \tag{232}$$

$n = 10$

$$\frac{945}{32a^{10}}\frac{\sqrt{\pi}}{a} = \int_{-\infty}^{\infty} (k-k_0)^{10} e^{-a^2(k-k_0)^2}\ dk, \tag{233}$$

The sequence of numbers $\{1, 3, 15, 105, 945\}$ fits the expansion $(2m+1)!/(m!2^m)$ for $m = 0, 1, 2, 3, 4$. The denominator has the series $\{2a^2, 4a^4, 8a^6, 16a^8, 32a^{10}\}$, which fits $(2a^2)^{(m+1)}$ for $m = 0, 1, 2, 3, 4$. Hence we have that,

$$\frac{(2m+1)!}{m!2^m} \frac{1}{(2a^2)^{m+1}} \frac{\sqrt{\pi}}{a} = \int_{-\infty}^{\infty} (k-k_0)^n e^{-a^2(k-k_0)^2} \, dk, \tag{234}$$

where $m = (n-2)/2$ and $n \geq 2$ and even. For $n \in \text{Odd}$, $\langle (k-k_0)^n \rangle = 0$.

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[1] We use symmetric Fourier transform coefficients $1, 1$, hence both forward and inverse FTs are multiplied by $1/2\pi$. A common alternative is $0, 1$ where the inverse FT is multiplied by the full $1/2\pi$.