**Some integrals with Gaussian wavepackets**

**1. Definition**

The normalized Gaussian wavepacket is defined as:

. (1)

Here, is the width parameter, is the center of the wavepacket, is the momentum of wavepacket.

**2. Overlap integral**

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Lets simplify:

.

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Thus,

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Pre-factor:

,

,

,

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The integral is:

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,

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Simplify:

.

So, the phase is:

Finally:

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When

.

And:

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Also:

.

So, that we recover the special result:

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**3. Transition dipole moment**

We will need an integral:

.

That is:

For , we recover the special result:

**4. Derivative coupling**

Differentiation of the ket function will yield:

So:

.

.

So:

For , we recover the special result:

**5. Kinetic energy matrix elements**

Double differentiation of the ket function will yield:

So:

So, we need the integral:

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That is:

Simplify:

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Imaginary terms:

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So, the overall imaginary term will be:

Now, onto the real terms:

Terms with

Common prefactor:

The rest:

So, the whole term is:

Terms without

Common prefactor:

The rest:

So, the term without is:

We also have the terms:

So, all together we get:

For , we recover the special result:

**6. Summary**

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Overlaps:

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Transition dipole moments:

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Couplings:

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Kinetic energy:

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