HW #7

1. Free particle path integral

a) Propagator

To simplify the notation, we write $t = t'' - t'$, $x = x'' - x'$ and work in 1D. Since $[x_i, p_j] = i\hbar\,\delta_{ij}$, we can just construct the 3D solution.

First of all, because the base kets evolve according to the "wrong sign" Schrödinger equation (see pp. 87−89),

$$|x', t'\rangle = e^{+iHt'/\hbar}\,|x', 0\rangle,\ \langle x'', t''| = \langle x'', 0|\,e^{-iHt''/\hbar}.$$

Therefore,

$$\langle x'', t''\,|\,x', t'\rangle = \langle x''\,|\,e^{-iH(t''-t')/\hbar}\,|\,x'\rangle = \int dp\,\langle x''\,|\,p\rangle\langle p\,|\,e^{-iHt/\hbar}\,|\,x'\rangle$$
$$= \int dp\,\frac{e^{ipx''/\hbar}}{(2\pi\hbar)^{1/2}}\,\langle p\,|\,e^{-i(p^2/2m)t/\hbar}\,|\,x'\rangle$$
$$= \int dp\,\frac{e^{ipx''/\hbar}}{(2\pi\hbar)^{1/2}}\,e^{-i(p^2/2m)t/\hbar}\,\frac{e^{-ipx'/\hbar}}{(2\pi\hbar)^{1/2}}$$
$$= \int dp\,\frac{e^{ipx/\hbar}}{2\pi\hbar}\,e^{-ip^2\,t/2m\hbar}$$
$$= \int dp\,\frac{1}{2\pi\hbar}\,\exp\!\left(-i\,\frac{t}{2m\hbar}\,\left(p - \frac{mx}{t}\right)^2 + i\,\frac{mx^2}{2\hbar t}\right)$$
$$= \frac{1}{2\pi\hbar}\sqrt{\frac{2\pi m\hbar}{it}}\;e^{imx^2/2\hbar t}$$
$$= \sqrt{\frac{m}{2\pi i\hbar t}}\;e^{imx^2/2\hbar t}$$

The analogous expression in three dimensions is simply

$$\left\langle \vec{x}'', t''\,\middle|\,\vec{x}', t'\right\rangle = \left(\frac{m}{2\pi i\hbar t}\right)^{3/2} e^{im\vec{x}^2/2\hbar t}\ .$$

b) Action in exponent

For the classical trajectory, the velocity is simply $\vec{v} = \frac{\vec{x}}{t}$, and hence the action is $S_c = \int \frac{1}{2}\,m\left(\frac{d\vec{x}}{dt}\right)dt = \frac{1}{2}\,m\left(\frac{\vec{x}}{t}\right)^2 t = \frac{m\vec{x}^2}{2t}$, and so the exponent of the propagator is indeed $(i S_c/\hbar)$.

c) Partition function

The partition function from statistical mechanics is

$$Z = \sum_{n=\square}^{\infty} \langle n \,|\, e^{-\beta H} \,|\, n \rangle,$$

where $| n \rangle$ can denote elements of any basis. Obviously, the Hamiltonian eigenstates themselves are generally most useful for calculating the sum directly; however, we can use the basis elements $| \vec{x} \rangle$ as well:

$$Z = \int d^3 x \left\langle \vec{x} \,\middle|\, e^{-\beta H} \,\middle|\, \vec{x} \right\rangle.$$

We observe that βH looks an awful lot like $i H t / \hbar$, except that the latter is purely imaginary whereas the former is purely real. Therefore, we define the "Euclidean" time τ by the analytic continuation $t \to -i \tau$ and get

$$Z = \int d^3 x \left\langle \vec{x} \,\middle|\, e^{-H \tau / \hbar} \,\middle|\, \vec{x} \right\rangle,$$

in which we set $\tau = \hbar \beta$, the thermal quantum timescale. Noting that $\langle \vec{x}, 0 \,|\, e^{-i H t / \hbar} = \langle \vec{x}, t \,|$ with "Minkowski" time in the Heisenberg picture (see part (a)), we get

$$Z = \int d^3 x \left\langle \vec{x}, -i \hbar \beta \,\middle|\, \vec{x}, 0 \right\rangle.$$

The conversion to Euclidean time is already complete, since $\vec{x}_f = \vec{x}_i = \vec{x}$. This is because if the topology of Minkowski time is an open line from $-\infty$ to ∞, the topology of Euclidean time must be a circle. Periodic functions of time become hyperbolic, and hyperbolic functions become periodic. Accordingly, in the exponent of the path integral, the action integral is now on a loop, and all trajectories return to their origin. Instead of computing the path integral, we can just convert our result for part (a) to get

$$Z = \int d^3 x \left(\frac{m}{2 \pi \hbar^2 \beta} \right)^{3/2} e^{-m\, 0 / 2 \hbar^2 \beta}$$

$$Z = V \left(\frac{m}{2 \pi \hbar^2 \beta} \right)^{3/2}$$

where V is the volume of the system. This is nothing but the single−particle partition function for the classical ideal gas in three dimensions, as expected.

It is interesting that changing from Minkowski time to Euclidean time would effect a change from a propagator that obeys the Schrödinger equation to a diffusion kernel that obeys the heat equation, and moreso that substituting $\hbar \beta$ for the Euclidean time yields the thermodynamic partition function per unit volume.

d) Superfluid transition temperature in He−4

In Euclidean time, the action integral is

$$S_E = \oint_0^{\hbar\beta} d\tau\, L = \oint_0^{\hbar\beta} d\tau\ \frac{m}{2}\left(\frac{d\vec{x}}{d\tau}\right)^2$$

where all paths are periodic, including particle exchange operations.

If one imagines Euclidean 1+1 spacetime as a cylinder, the trajectories of two umolested particles are just single loops around. However, if we switch the particles, the trajectories cross −− the trajectory starting at particle 1 attaches to the start of the trajectory of particle 2 after wrapping around the cylinder, and vice−versa. In order for this switching operation to be undone (i.e., for the trajectories to be closed), the trajectories have to make *one more* trip around, to connect to where they started originally. So, with a switching operation, each particle has an average of one extra loop in calculating the action.

Naively, one might simply make the thermal quantum substitutions λ (the thermal de Broglie wavelength) and $\hbar\beta$ for $\left|d\vec{x}\right| = dx$ and $d\tau$ respectively. While this makes sense for $d\tau$, one must be careful with dx. Trying it, one would find the result $S_E \sim N\hbar$, where we define N to be the number of loops around the Euclidean spacetime cylinder, with all the other constants cancelling. That is, it would quantize "too far" −− we need to retain some length scale that’s relevant to the inter−particle dynamics that changes the normal fluid to a superfluid.

Generally, the relevant length scale is the "mean free path" l_f, which is the average distance a particle travels between collisions. In the low temperature regime where the particles are evenly distributed in Boltzmann fashion as in part (c), multiple bosons would pile up as a condensate. That is, many particles would share the same ground state wavefunction; moreover, the classical interactions between particles would be sphere−like, with no "screening" effects (and ignoring mean field effects). In this case,

$$l_f \approx \left(\sqrt{2}\, n \times \sigma\right)^{-1} \approx \left(\sqrt{2}\, n \times \frac{\pi n^{-2/3}}{4}\right)^{-1} \approx \frac{2^{3/2}}{\pi} n^{-1/3}$$

where n is the number density, and the factor of $\sqrt{2}$ comes from the Maxwell−like distribution of particle velocities. (If a particle of interest were much faster than all the other particles, we would just use $(n \times \sigma)^{-1}$, which is easy to see geometrically.) Note we just substituted $n^{-1/3}$ for the cross−sectional diameter.

Let us try $dx \approx l_f$:

$$S_E \approx \oint_0^{\hbar\beta} d\tau\ \frac{m}{2}\left(\frac{l_f}{\hbar\beta}\right)^2 = \frac{m}{2}\left(\frac{l_f}{\hbar\beta}\right)^2 \oint_0^{\hbar\beta} d\tau$$

$$= \frac{m}{2}\left(\frac{l_f}{\hbar\beta}\right)^2 N\hbar\beta = \frac{m}{2}\ \frac{8}{\pi^2 n^{2/3}}\ \frac{1}{\hbar\beta} N = \frac{4m}{\pi^2 n^{2/3}\hbar\beta} N\ .$$

Now, we want the temperature at which the change in S_E is $\hbar$ with each additional loop:

$$\Delta S_E = \frac{4m}{\pi^2 n^{2/3}\hbar\beta} \simeq \hbar \Longrightarrow T_\lambda \simeq \frac{\pi^2\hbar^2 n^{2/3}}{4k_B m} = \frac{\pi^2\hbar^2\rho^{2/3}}{4k_B m^{5/3}}$$

where ρ is the mass density at the superfluid transition T_λ. Let us compute it, with a figure of 7.798 lb/ft^3 for the mass density of liquid He−4 @ 4 K (from the liquid helium safety data sheet; 4.22 K is the boiling point according to Wikipedia):

```
π² ℏ² ρ^(2/3) / (4 k_B m^(5/3)) /. {k_B -> 1.38 * 10^-23, ℏ → 1.055 * 10^-34, m → 4 * 1.66 * 10^-27, ρ → 7.798 * 16}
```

$$\frac{\pi^2\,\hbar^2\,\rho^{2/3}}{4\,k_B\,m^{5/3}}$$

```
2.1183
```

This result is embarrassingly close to the measured value of 2.1768 K (Wikipedia), for having used such hand−wavy arguments!

2. Propagator of harmonic oscillator

a) Propagator with energy eigenvalues

As in 1(a) above,

$$K = \langle x_f, t_f \mid x_i, t_i \rangle = \langle x_f, t_i \mid e^{-i H (t_f - t_i)/\hbar} \mid x_i, t_i \rangle .$$

We can insert the unity operator, on the basis of Hamiltonian eigenstates $| n \rangle$:

$$\langle x_f, t_f \mid x_i, t_i \rangle = \sum_{n=0}^{\infty} \langle x_f, t_i \mid e^{-i H (t_f - t_i)/\hbar} \mid n \rangle \langle n \mid x_i, t_i \rangle$$
$$= \sum_{n=0}^{\infty} \langle x_f, t_i \mid n \rangle \langle n \mid x_i, t_i \rangle e^{-i E_n (t_f - t_i)/\hbar}$$
$$= \sum_{n=0}^{\infty} \psi_n(x_f)^* \psi_n(x_i) e^{-i E_n (t_f - t_i)/\hbar} .$$

Making the usual substitution $t_f - t_i = -i\tau$, we obtain the desired result

$$K = \sum_{n=0}^{\infty} \psi_n(x_f)^* \psi_n(x_i) e^{-E_n \tau/\hbar} .$$

b) Leading behavior

We implement the harmonic oscillator propagator and make the substitution for $t_f - t_i = -i\tau = i\ln(\epsilon)/\omega$:

```
kho = Sqrt[(m ω)/(2 π I ℏ Sin[ω (t - t0)])] Exp[((I m ω)/(2 ℏ Sin[ω (t - t0)])) ((x^2 + x0^2) Cos[ω (t - t0)] - 2 x x0)] /.
   (t - t0) → I Log[ϵ] / ω;
```

As $\tau \to \infty$, $\epsilon \to 0$, so we can expand it around $\epsilon = 0$:

```
Series[kho, {ϵ, 0, 1}]
```

$$\frac{e^{-\frac{m x^2 \omega}{2\hbar} - \frac{m x0^2 \omega}{2\hbar}} \sqrt{\frac{m\omega}{\hbar}} \sqrt{\epsilon}}{\sqrt{\pi}} + O[\epsilon]^{3/2}$$

We see that the leading order is $\epsilon^{1/2}$ as expected.

c) Expansion to arbitrary order

Expand the propagator to order $10 + 1/2 = 21/2$:

```
khos = Series[kho, {ϵ, 0, 11}];
```

Extract the wavefunctions:

```
khos0 = Simplify[(SeriesCoefficient[khos, 1] /. x0 → x)^(1/2),
  Assumptions → {ℏ > 0, m > 0, ω > 0, x ∈ Reals}]
khos5 = Simplify[(SeriesCoefficient[khos, 11] /. x0 → x)^(1/2),
  Assumptions → {ℏ > 0, m > 0, ω > 0, x ∈ Reals}]
khos10 = Simplify[(SeriesCoefficient[khos, 21] /. x0 → x)^(1/2),
  Assumptions → {ℏ > 0, m > 0, ω > 0, x ∈ Reals}]
```

$$\frac{e^{-\frac{m x^2 \omega}{2 \hbar}} \left(\frac{m \omega}{\hbar}\right)^{1/4}}{\pi^{1/4}}$$

$$\frac{e^{-\frac{m x^2 \omega}{2 \hbar}} \left(\frac{m \omega}{\hbar}\right)^{3/4} \mathrm{Abs}[15 \hbar^2 x - 20 \hbar m x^3 \omega + 4 m^2 x^5 \omega^2]}{2 \sqrt{15} \hbar^2 \pi^{1/4}}$$

$$\frac{1}{720 \sqrt{7} \pi^{1/4}} \left(e^{-\frac{m x^2 \omega}{2 \hbar}} \left(\frac{m \omega}{\hbar^{21}}\right)^{1/4} \mathrm{Abs}[945 \hbar^5 - 9450 \hbar^4 m x^2 \omega + 12600 \hbar^3 m^2 x^4 \omega^2 - 5040 \hbar^2 m^3 x^6 \omega^3 + 720 \hbar m^4 x^8 \omega^4 - 32 m^5 x^{10} \omega^5]\right)$$

So we find the wavefunctions:

$$\psi k0 = \frac{e^{-\frac{m x^2 \omega}{2 \hbar}} \left(\frac{m \omega}{\hbar}\right)^{1/4}}{\pi^{1/4}};$$

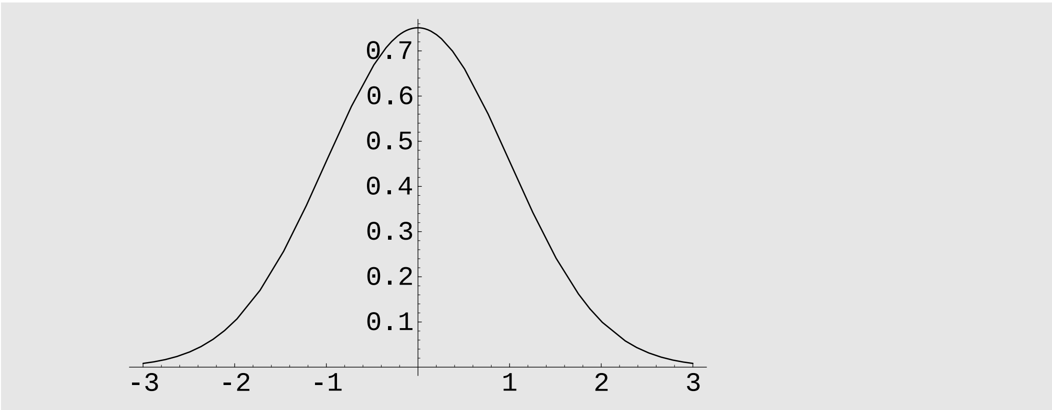
$$\psi k5 = \frac{e^{-\frac{m x^2 \omega}{2 \hbar}} \left(\frac{m \omega}{\hbar}\right)^{3/4} (15 \hbar^2 x - 20 \hbar m x^3 \omega + 4 m^2 x^5 \omega^2)}{2 \sqrt{15} \hbar^2 \pi^{1/4}};$$

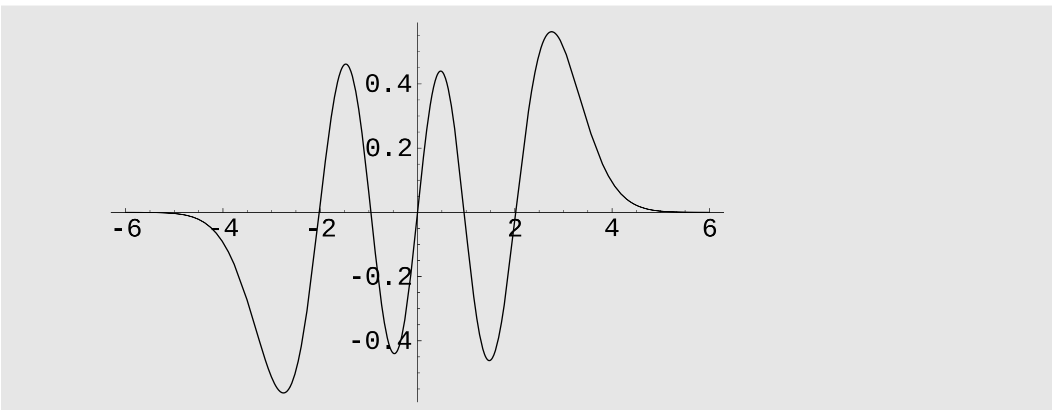
$$\psi k10 = \frac{1}{720 \sqrt{7} \pi^{1/4}} \left(e^{-\frac{m x^2 \omega}{2 \hbar}} \left(\frac{m \omega}{\hbar^{21}}\right)^{1/4} (945 \hbar^5 - 9450 \hbar^4 m x^2 \omega + 12600 \hbar^3 m^2 x^4 \omega^2 - 5040 \hbar^2 m^3 x^6 \omega^3 + 720 \hbar m^4 x^8 \omega^4 - 32 m^5 x^{10} \omega^5)\right);$$

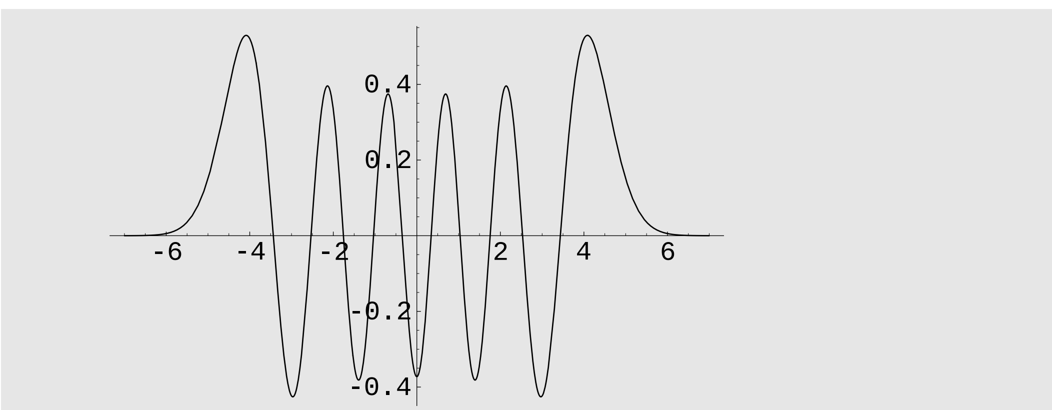
d) Graph and check normalization

Let us plot our wavefunctions:

```
nums = {m → 1, ℏ → 1, ω → 1};
Plot[ψx0 /. nums, {x, -3, 3}];
Plot[ψx5 /. nums, {x, -6, 6}];
Plot[ψx10 /. nums, {x, -7, 7}];
```







And show that they're normalized to 1:

```
Integrate[ψk0^2, {x, -∞, ∞}, Assumptions -> {ℏ > 0, m > 0, ω > 0}]
Integrate[ψk5^2, {x, -∞, ∞}, Assumptions -> {ℏ > 0, m > 0, ω > 0}]
Integrate[ψk10^2, {x, -∞, ∞}, Assumptions -> {ℏ > 0, m > 0, ω > 0}]
```

```
1
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1
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1
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3. Discretized HO path integral [optional]

See path integral notes pp. 15−19.