Differential Equations of Mathematical Physics
(APM 351 Y)

2013–2014
Solutions 17
(2014.02.27)

Quantum Mechanics

Homework Problems

54. The energy functional for the quantum harmonic oscillator (24 points)

Define the average energy

$$\mathbb{E}_{\varphi}(H) := \int_{\mathbb{R}} \mathrm{d}x \, \left(\frac{1}{2m} \left| \varphi'(x) \right|^2 + V(x) \left| \varphi(x) \right|^2 \right) =: \mathbb{E}_{\varphi}\big(-\tfrac{1}{2m}\partial_x^2\big) + \mathbb{E}_{\varphi}(V)$$

associated to the hamiltonian $H = -\frac{1}{2m}\partial_x^2 + V$ and $\psi \in \mathcal{S}(\mathbb{R})$, seen as the sum of kinetic energy $\mathbb{E}_{\varphi}\big(-\frac{1}{2m}\partial_x^2\big)$ and potential energy $\mathbb{E}_{\varphi}(V)$.

Consider the case of the harmonic oscillator where $V(x) = \frac{m}{2}\omega^2 x^2$ is the potential energy and $\omega > 0$ the characteristic frequency of the oscillator. Moreover, define the family of scaled Gaußians $\varphi_\lambda(x) := \pi^{-1/4} \sqrt{\lambda} \, \mathrm{e}^{-\frac{\lambda^2}{2}x^2}$, $\lambda > 0$.

(i) Determine the expected value of the energy $E(\lambda) := \mathbb{E}_{\varphi_\lambda}(H)$ as a function of λ.

(ii) Find the λ_{min} which minimizes $E(\lambda)$. Give the minimizing wavefunction $\varphi_0 := \varphi_{\lambda_{\text{min}}}$.

(iii) For which λ is the expected value of the kinetic energy small? What about the potential energy? Interpret your results.

(iv) Determine $E_0 \in \mathbb{R}$ so that φ_0 from (ii) satisfies the eigenvalue equation

$$H\varphi_0 = E_0 \, \varphi_0.$$

Solution:

(i) To compute $\mathcal{E}(\varphi_\lambda)$ we need the derivative of φ_λ:

$$\frac{\mathrm{d}}{\mathrm{d}x}\varphi_\lambda(x) = \pi^{-1/4}\sqrt{\lambda}\,(-\lambda^2 x)\mathrm{e}^{-\frac{\lambda^2}{2}x^2} = (-\lambda^2 x)\varphi_\lambda(x) \qquad [1]$$

Plugged into $\mathcal{E}(\varphi_\lambda)$ we obtain

$$\begin{aligned} E(\lambda) : &= \mathbb{E}_{\varphi_\lambda}(H) \overset{[1]}{=} \int_{\mathbb{R}} \mathrm{d}x \, \left(\frac{1}{2m} \left| \varphi_\lambda'(x) \right|^2 + \frac{m}{2}\omega^2 x^2 \left| \varphi_\lambda(x) \right|^2 \right) \\ &= \int_{\mathbb{R}} \mathrm{d}x \, \left(\frac{1}{2m} \left| (-\lambda^2 x) \, \pi^{-1/4}\sqrt{\lambda} \, \mathrm{e}^{-\frac{\lambda^2}{2}x^2} \right|^2 + \frac{m}{2}\omega^2 x^2 \left| \pi^{-1/4}\sqrt{\lambda} \, \mathrm{e}^{-\frac{\lambda^2}{2}x^2} \right|^2 \right) \\ &\overset{[1]}{=} \frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} \mathrm{d}x \, \lambda \frac{1}{2m} \big(\lambda^4 + m^2\omega^2\big) \, x^2 \, \mathrm{e}^{-\lambda^2 x^2} . \end{aligned}$$

We make a change of variables and obtain the Gauß integral after partial integration:

$$\begin{aligned}
E(\lambda) &\overset{[1]}{=} \frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} \mathrm{d}y \, \frac{1}{\lambda} \cdot \lambda \frac{1}{2m} \big(\lambda^4 + m^2\omega^2\big) \, \lambda^{-2} y^2 \, \mathrm{e}^{-y^2} \\
&\overset{[1]}{=} \frac{1}{\sqrt{\pi}} \underbrace{\frac{1}{2m} \big(\lambda^2 + m^2\omega^2\lambda^{-2}\big)}_{=:C(\lambda)} \cdot 2 \int_0^\infty \mathrm{d}y \, y \cdot y \, \mathrm{e}^{-y^2} \\
&\overset{[1]}{=} \frac{2}{\sqrt{\pi}} C(\lambda) \Big[y \cdot \big(-\tfrac{1}{2}\mathrm{e}^{-y^2}\big) \Big]_0^\infty - \frac{2}{\sqrt{\pi}} C(\lambda) \int_0^\infty \mathrm{d}y \, 1 \cdot \big(-\tfrac{1}{2}\mathrm{e}^{-y^2}\big) \\
&= 0 + \frac{1}{\sqrt{\pi}} C(\lambda) \int_0^\infty \mathrm{d}y \, \mathrm{e}^{-y^2} \overset{[1]}{=} \frac{1}{\sqrt{\pi}} C(\lambda) \int_0^\infty \mathrm{d}\xi \, \frac{1}{2} \xi^{-1/2} \, \mathrm{e}^{-\xi} \\
&\overset{[1]}{=} \frac{1}{2\sqrt{\pi}} C(\lambda) \, \Gamma\big(\tfrac{1}{2}\big) \overset{[1]}{=} \frac{1}{4m} \big(\lambda^2 + m^2\omega^2\lambda^{-2}\big)
\end{aligned}$$

(ii) We compute the first two derivatives of the function $E(\lambda)$:

$$\begin{aligned}
E'(\lambda) &= \frac{1}{4m} \big(2\lambda - 2m^2\omega^2\lambda^{-3}\big) = \frac{1}{2m} \big(\lambda - m^2\omega^2\lambda^{-3}\big) \\
E''(\lambda) &= \frac{1}{2m} \big(1 + 3m^2\omega^2\lambda^{-4}\big) > 0 \qquad [1]
\end{aligned}$$

Hence, the expected value of the energy is a convex function of λ. We determine the local extrema by setting the derivative 0:

$$E'(\lambda) = \frac{1}{2m} \big(\lambda - m^2\omega^2\lambda^{-3}\big) \overset{!}{=} 0 \qquad [1]$$

Consequently, $\lambda^4 = m^2\omega^2$, so that $\lambda_c = \sqrt{m\omega}$ [1]. At this point,

$$E(\lambda_c) = \frac{1}{4m} \left(m\omega + m^2\omega^2 \cdot \frac{1}{m\omega} \right) = \tfrac{1}{4} (\omega + \omega) = \tfrac{\omega}{2}. \qquad [1]$$

Since $E(\lambda)$ tends to ∞ for large and small λ, $\lim_{\lambda \searrow 0} E(\lambda) = \infty = \lim_{\lambda \to \infty} E(\lambda)$, the point $\big(\lambda_{\text{min}}, E(\lambda_{\text{min}})\big) = \big(\sqrt{m\omega}, \frac{\omega}{2}\big)$ is necessarily a *global minimum* [1] and

$$\varphi_0(x) = \varphi_{\sqrt{m\omega}}(x) = \sqrt[4]{\frac{m\omega}{\pi}} \, \mathrm{e}^{-\frac{m\omega x^2}{2}} \qquad [1]$$

the state of minimal energy.

(iii) Looking at the computation in (i), we immediately see

$$\begin{aligned}
\mathbb{E}_{\varphi_\lambda}\big(-\tfrac{1}{2m}\partial_x^2\big) &= \frac{1}{4m}\lambda^2 \\
\mathbb{E}_{\varphi_\lambda}(V) &= \frac{m}{4}\omega^2\lambda^{-2}. \qquad [1]
\end{aligned}$$

The average kinetic energy is small if $\lambda \ll 1$ is small [1]; $\lambda \ll 1$ means that the wave function is flat and spread out, the particle is delocalized [1].

Conversely, the average potential energy is small if $\lambda \gg 1$ [1]; then φ_λ is sharply peaked around $x = 0$ and the particle is well-localized [1].

(iv) We plug the second derivative of φ_0,

$$\begin{aligned}\varphi_0'(x) &= \frac{\mathrm{d}}{\mathrm{d}x}\sqrt[4]{\frac{m\omega}{\pi}}\,\mathrm{e}^{-\frac{m\omega x^2}{2}} = -\sqrt[4]{\frac{m\omega}{\pi}} m\omega\, x\,\mathrm{e}^{-\frac{m\omega x^2}{2}} = -m\omega\, x\,\varphi_0(x)\\ \varphi_0''(x) &= -\sqrt[4]{\frac{m\omega}{\pi}} m\omega\,\mathrm{e}^{-\frac{m\omega x^2}{2}} + \sqrt[4]{\frac{m\omega}{\pi}}(-m\omega\, x)^2\,\mathrm{e}^{-\frac{m\omega x^2}{2}}\\ &= \sqrt[4]{\frac{m\omega}{\pi}} m\omega\left(m\omega\, x^2 - 1\right)\mathrm{e}^{-\frac{m\omega x^2}{2}} = m\omega\left(m\omega\, x^2-1\right)\varphi_0(x), \qquad [1]\end{aligned}$$

into the left-hand side of $H\varphi_0$ and obtain

$$\begin{aligned}-\frac{1}{2m}\varphi_0''(x) + \frac{m}{2}\omega^2 x^2\,\varphi_0(x) &\overset{[1]}{=} \left(-\frac{1}{2m}m\omega\left(m\omega\, x^2-1\right) + \frac{m}{2}\omega^2 x^2\right)\varphi_0(x)\\ &\overset{[1]}{=} \tfrac{\omega}{2}\,\varphi_0(x) + \tfrac{1}{2}\left(-m\omega^2 + m\omega^2\right)x^2\,\varphi_0(x) \overset{[1]}{=} \tfrac{\omega}{2}\,\varphi_0(x).\end{aligned}$$

That means $E_0 = \frac{\omega}{2} = E\left(\sqrt{m\omega}\right)$ [1].

55. The free relativistic Schrödinger operator

Consider the free relativistic Schrödinger operator $H := \sqrt{m^2 - \Delta_x}$ on $L^2(\mathbb{R}^d)$ defined as in problem 4 of Test 2.

(i) Compute $\sigma(H)$.

(ii) Determine the nature of the spectrum, i. e. determine $\sigma_{\text{ess}}(P)$, $\sigma_{\text{disc}}(P)$, $\sigma_{\text{cont}}(P)$ and $\sigma_{\text{p}}(P)$.

(iii) Are the eigenfunctions elements of the Hilbert space?

Solution:

(i) By definition, the operator is unitarily equivalent to the operator of multiplication by $T(\xi) = \sqrt{m^2 + \xi^2}$, and hence, $\sigma(H) = \operatorname{ran} T = [0, +\infty)$.

(ii) The function T is nowhere locally constant, and thus, the spectrum is purely essential and purely continuous,

$$\sigma(H) = \sigma_{\text{ess}}(H) = \sigma_{\text{cont}}(H),$$
$$\sigma_{\text{p}}(H) = \sigma_{\text{disc}}(H) = \emptyset.$$

(iii) The eigenfunctions of H are plane waves $\mathrm{e}^{+\mathrm{i}\xi \cdot x}$ which are not square integrable.

56. The Wigner transform: fundamental properties

The Wigner transform of a Schwartz function $\psi \in \mathcal{S}(\mathbb{R})$ is defined as

$$\big(\mathcal{W}(\psi)\big)(x,\xi) := \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}y \, \mathrm{e}^{-\mathrm{i}y\,\xi} \, \overline{\psi\big(x - \tfrac{\varepsilon}{2}y\big)} \, \psi\big(x + \tfrac{\varepsilon}{2}y\big)$$

where x is position and ξ is momentum.

(i) Show that $\mathcal{W}(\psi)$ is a real-valued function on phase space $\mathbb{R}^2$.

(ii) Compute the marginals of the Wigner transform,

$$\int_{\mathbb{R}} \mathrm{d}x \, \big(\mathcal{W}(\psi)\big)(x,\xi), \qquad \int_{\mathbb{R}} \mathrm{d}\xi \, \big(\mathcal{W}(\psi)\big)(x,\xi), \qquad \int_{\mathbb{R}^2} \mathrm{d}x \, \mathrm{d}\xi \, \big(\mathcal{W}(\psi)\big)(x,\xi).$$

(iii) Show $\big(\mathcal{W}(T_{x'}\psi)\big)(x,\xi) = \big(\mathcal{W}(\psi)\big)(x - x',\xi)$ where $(T_{x'}\psi)(x) := \psi(x - x')$.

Solution:

(i) We have to show $\overline{\mathcal{W}(\psi)} = \mathcal{W}(\psi)$:

$$\begin{aligned}
\overline{\big(\mathcal{W}(\psi)\big)(x,\xi)} &= \overline{\frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}y \, \mathrm{e}^{-\mathrm{i}y\,\xi} \, \overline{\psi\big(x - \tfrac{\varepsilon}{2}y\big)} \, \psi\big(x + \tfrac{\varepsilon}{2}y\big)} \\
&= \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}y \, \mathrm{e}^{+\mathrm{i}y\cdot\xi} \, \psi\big(x - \tfrac{\varepsilon}{2}y\big) \, \overline{\psi\big(x + \tfrac{\varepsilon}{2}y\big)} \\
&= \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}y \, \mathrm{e}^{-\mathrm{i}y\cdot\xi} \, \psi\big(x + \tfrac{\varepsilon}{2}y\big) \, \overline{\psi\big(x - \tfrac{\varepsilon}{2}y\big)} = \big(\mathcal{W}(\psi)\big)(x,\xi).
\end{aligned}$$

(ii) If we take the marginals with respect to x, we get

$$\begin{aligned}
\int_{\mathbb{R}} \mathrm{d}x \, \big(\mathcal{W}(\psi)\big)(x,\xi) &= \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}x \int_{\mathbb{R}} \mathrm{d}y \, \mathrm{e}^{-\mathrm{i}y\,\xi} \, \overline{\psi\big(x - \tfrac{\varepsilon}{2}y\big)} \, \psi\big(x + \tfrac{\varepsilon}{2}y\big) \\
&= \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}x' \int_{\mathbb{R}} \mathrm{d}y \, \mathrm{e}^{-\mathrm{i}y\,\xi} \, \overline{\psi(x')} \, \psi(x' + \varepsilon y) \\
&= \frac{\varepsilon^{-d}}{2\pi} \int_{\mathbb{R}} \mathrm{d}x' \int_{\mathbb{R}} \mathrm{d}y' \, \mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}(y' - x')\,\xi} \, \overline{\psi(x')} \, \psi(y') \\
&= \varepsilon^{-d} \, \big|(\mathcal{F}\psi)(\xi/\varepsilon)\big|^2.
\end{aligned}$$

The other marginal can be obtained analogously,

$$\int_{\mathbb{R}} \mathrm{d}\xi \, \big(\mathcal{W}(\psi)\big)(x,\xi) = |\psi(x)|^2.$$

The above calculations show

$$\int_{\mathbb{R}^2} \mathrm{d}x \, \mathrm{d}\xi \, \big(\mathcal{W}(\psi)\big)(x,\xi) = \|\psi\|^2 .$$

(iii)

$$\begin{aligned}
\big(\mathcal{W}(T_y\psi)\big)(x,\xi) &= \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}y \, \mathrm{e}^{-\mathrm{i}y\,\xi} \, \overline{(T_{x'}\psi)\big(x - \tfrac{\varepsilon}{2}y\big)} \, (T_{x'}\psi)\big(x + \tfrac{\varepsilon}{2}y\big) \\
&= \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}y \, \mathrm{e}^{-\mathrm{i}y\,\xi} \, \overline{\psi\big(x - x' - \tfrac{\varepsilon}{2}y\big)} \, \psi\big(x - x' + \tfrac{\varepsilon}{2}y\big) \\
&= \big(\mathcal{W}(\psi)\big)(x - x',\xi)
\end{aligned}$$

57. The Wigner transform: computations of Wigner transforms

Define the Wigner transform as in problem 56 but set $\varepsilon = 1$.

(i) Compute the Wigner transform of $\psi(x) = \mathrm{e}^{+\mathrm{i}\xi_c\, x}\, \mathrm{e}^{-\frac{x^2}{2b^2}}$. Explain at what point in $\mathbb{R}^2$ the Wigner transformed function takes its maximum.

(ii) Which roles do the parameters b and ξ_c from part (i) play? What does the Wigner transform of $\psi(x - x_c)$ look like?

(iii) Compute the Wigner transform of $\varphi(x) = x\, \mathrm{e}^{-\frac{x^2}{4}}$.

(iv) Can the Wigner transform be interpreted as a classical state?

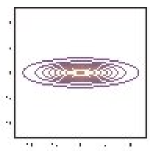
Solution:

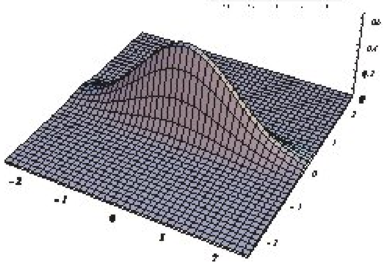
(i) We plug ψ into the definition of the Wigner transform and obtain:

$$\begin{aligned}
\big(\mathcal{W}(\psi)\big)(x,\xi) &= \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}y\, \mathrm{e}^{-\mathrm{i}\xi\, y}\, \overline{\psi\big(x - \tfrac{y}{2}\big)}\, \psi\big(x + \tfrac{y}{2}\big) \\
&= \frac{1}{2\pi} \int_{\mathbb{R}^d} \mathrm{d}y\, \mathrm{e}^{-\mathrm{i}\xi\, y}\, \mathrm{e}^{-\mathrm{i}\xi_c\, (x - \frac{y}{2})}\, \mathrm{e}^{-\frac{(x-\frac{y}{2})^2}{2b^2}}\, \mathrm{e}^{+\mathrm{i}\xi_c\, (x + \frac{y}{2})}\, \mathrm{e}^{-\frac{(x+\frac{y}{2})^2}{2b^2}} \\
&= \frac{1}{2\pi} \int_{\mathbb{R}^d} \mathrm{d}y\, \mathrm{e}^{-\mathrm{i}(\xi_c - \xi)\, y}\, \mathrm{e}^{-\frac{x^2}{b^2}}\, \mathrm{e}^{-\frac{y^2}{4b^2}} \\
&= \mathrm{e}^{-\frac{x^2}{b^2}} \left(2\pi\, (2b^2)^{-1}\right)^{-1/2} \mathrm{e}^{-\frac{x^2}{2}}\, \mathrm{e}^{-\frac{(\xi-\xi_c)^2\, 2b^2}{2}} \\
&= \frac{b}{\sqrt{\pi}}\, \mathrm{e}^{-\frac{x^2}{2}}\, \mathrm{e}^{-b^2 (\xi - \xi_c)^2}
\end{aligned}$$

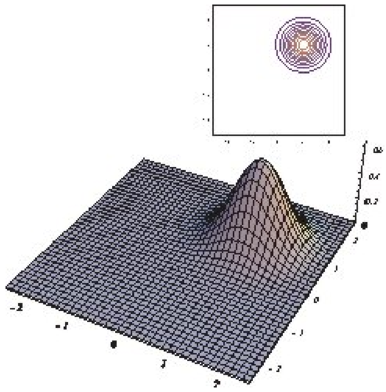
The wave packet is centered around the point $(0, \xi_c)$ in phase space.

(ii) The parameter b quantifies the *width* of the wave packet in real space. Since the widths in real and momentum space are inverses of one another, the state looks as follows:





ξ_c gives the position of the maximum in momentum space. The prefactor $\mathrm{e}^{-\mathrm{i}\xi_c \cdot x}$ shifts the wave packet in momentum space by ξ_c. Replacing x by $x - x_c$ translates the wave packet in real space:



(iii)

$$\begin{aligned}
\big(\mathcal{W}(\varphi)\big)(x,\xi) &= \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}y\, \mathrm{e}^{-\mathrm{i}y\cdot\xi}\,\overline{\varphi\big(x-\tfrac{y}{2}\big)}\,\varphi\big(x+\tfrac{y}{2}\big) \\
&= \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}y\, \mathrm{e}^{-\mathrm{i}y\cdot\xi}\,\big(x-\tfrac{y}{2}\big)\,\big(x+\tfrac{y}{2}\big)\,\mathrm{e}^{-\frac{1}{4}[(x-\frac{y}{2})^2+(x+\frac{y}{2})^2]} \\
&= 2\mathrm{e}^{-\frac{x^2}{2}}\,\frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}y\, \mathrm{e}^{-\mathrm{i}y\cdot 2\xi}\,(x^2-y^2)\,\mathrm{e}^{-\frac{y^2}{2}} \\
&= \pi^{-1}\,\mathrm{e}^{-\frac{x^2}{2}}\,\Big(x^2\mathrm{e}^{-2\xi^2}+\tfrac{1}{4}\partial_\xi^2\big(\mathrm{e}^{-2\xi^2}\big)\Big) \\
&= \pi^{-1}\Big(x^2+(2\xi)^2-1\Big)\,\mathrm{e}^{-2x^2}\mathrm{e}^{-2\xi^2} \ngeq 0.
\end{aligned}$$

58. Ground state of the cut off Lenard-Jones potential

Consider the hamiltonian $H_\lambda = -\partial_x^2 + \lambda V$, $\lambda > 0$, for the cut off Lenard-Jones potential

$$V(x) = \begin{cases} \frac{1}{|x|^{12}} - \frac{1}{|x|^6} & |x| \geq 1 \\ 0 & |x| < 1 \end{cases}$$

in one dimension.

(i) Show that there exists a $\lambda_0 > 0$ such that for all $0 < \lambda < \lambda_0$ the hamiltonian H_λ has a unique bound state of energy $E_\lambda < 0$.

(ii) Compute E_λ to leading order in λ.

Solution:

(i) The function V is non-positive, has no singularity and decays as $|x|^{-6}$ for large $|x|$. Consequently, $V, x^2 V \in L^1(\mathbb{R})$ and Theorem 9.3.7 applies, i. e. there exists $\lambda_0 > 0$ so that H_λ has a unique bound state of energy $E_\lambda < 0$.

(ii) Equation (9.3.3) gives an explicit estimate on the value of $E_\lambda = -\frac{\lambda^2}{4} \|V\|_{L^1(\mathbb{R})}^2 + \mathcal{O}(\lambda^4)$ to leading order, and hence, we need to compute

$$\begin{aligned} \int_{\mathbb{R}} \mathrm{d}x \, |V(x)| &= -2 \int_1^\infty \mathrm{d}x \, \left(\frac{1}{|x|^{12}} - \frac{1}{|x|^6} \right) = -2 \left[\frac{x^{-11}}{-11} - \frac{x^{-5}}{-5} \right]_1^\infty \\ &= \frac{2}{5} - \frac{2}{11} = \frac{12}{55} \approx 0.218. \end{aligned}$$

Plugged into equation (9.3.3) then yields

$$E_\lambda = -\lambda^2 \frac{6^2}{55^2} + \mathcal{O}(\lambda^4) \approx 0.0119 \cdot \lambda^2 + \mathcal{O}(\lambda^4).$$