SOLUTIONS for Homework #4

1. It is convenient to use the vector form writing all vectors $\mathbf{V}$ in terms of their Cartesian components V_i. The basic commutator is that between the components of the position vector $\hat{x}_i$ and those of the momentum vector $\hat{p}_i$,

$$[\hat{p}_i, \hat{x}_j] = -i\hbar\delta_{ij}. \tag{1}$$

The components of the orbital momentum operator $\hat{\mathbf{L}}$ are

$$\hat{L}_i = (\hat{\mathbf{r}} \times \hat{\mathbf{p}})_i = \epsilon_{ijk}\hat{x}_j\hat{p}_k, \tag{2}$$

where ϵ_{ijk} is the fully antisymmetric tensor which has the nonzero components only if all three indices are different, and these nonzero components are equal to 1 for the right-hand order of indices (123, 231, and 312), and -1 for the left-hand order (213, 321, and 132); as always in such cases, the summation over twice repeated Cartesian indices (in our case j and k) is implied and not indicated explicitly. Note that in this expression the order of coordinate and momentum operator does not matter because the vector product contains only the products of *different* components of coordinate and momentum, and the latter commute, eq. (1).

From eq. (1) it follows for arbitrary functions $f(\hat{\mathbf{r}})$ or $g(\hat{\mathbf{p}})$ that

$$[\hat{p}_i, f(\hat{\mathbf{r}})] = -i\hbar\frac{\partial f}{\partial \hat{x}_i}, \quad [\hat{x}_i, g(\hat{\mathbf{p}})] = i\hbar\frac{\partial g}{\partial \hat{p}_i}. \tag{3}$$

Take, for example a scalar function of momentum $g(\hat{\mathbf{p}}^2)$. Since the momentum components commute among themselves,

$$[\hat{L}_i, g(\hat{\mathbf{p}}^2)] = \epsilon_{ijk}[\hat{x}_j\hat{p}_k, g(\hat{\mathbf{p}}^2)] = \epsilon_{ijk}[\hat{x}_j, g(\hat{\mathbf{p}}^2)]\hat{p}_k. \tag{4}$$

The gradient of any scalar function has a radial direction in corresponding space:

$$\frac{\partial}{\partial p_j}g(\mathbf{p}^2) = \frac{\partial g}{\partial p}\frac{p_j}{p}. \tag{5}$$

Therefore we come to

$$[\hat{L}_i, g(\hat{\mathbf{p}}^2)] = \epsilon_{ijk}\hat{p}_j\hat{p}_k \times \text{function}(\hat{\mathbf{p}}^2) = 0, \tag{6}$$

since the result would be the i-th component of the vector product of the momentum vector by itself, and such a product is equal to zero (this follows formally from the antisymmetry of ϵ_{ijk} which is contracted with the symmetric tensor p_jp_k). The same conclusion holds for a scalar function of coordinates. The physical reason for the disappearance of the commutators of the orbital momentum with scalars is in the fact that, as we will see later, the orbital momentum is the *generator of spatial rotations*, and scalar functions do not change (are *invariant*) under rotations.

Now we immediately see that the operator of kinetic energy

$$\hat{K} = \frac{\hat{\mathbf{p}}^2}{2m} \tag{7}$$

is a scalar function of the momentum vector and therefore commutes with the orbital momentum. For the operator $U(\hat{\mathbf{r}})$ we obtain in a similar way

$$[\hat{L}_i, U(\hat{\mathbf{r}})] = \epsilon_{ijk}\hat{x}_j[\hat{p}_k, U(\hat{\mathbf{r}}] = -i\hbar\epsilon_{ijk}\hat{x}_j\nabla_k U(\hat{\mathbf{r}}) = -i\hbar\left(\hat{\mathbf{r}} \times \nabla\hat{U}\right)_i. \tag{8}$$

Again, for a potential with central symmetry, $U = U(r)$, its gradient is directed radially, and the vector product in (8) vanishes.

Since the orbital momentum operator its time independent, the Ehrenfest equation of motion for its expectation value is

$$\frac{d}{dt}\langle\hat{\mathbf{L}}\rangle = \frac{1}{i\hbar}\langle[\hat{\mathbf{L}}, \hat{H}]\rangle. \tag{9}$$

The commutator with kinetic energy disappears, and the result is

$$\frac{d}{dt}\langle\hat{\mathbf{L}}\rangle = -\langle(\hat{\mathbf{r}} \times \nabla\hat{U})\rangle = \langle(\hat{\mathbf{r}} \times \hat{\mathbf{F}})\rangle, \tag{10}$$

where $\hat{\mathbf{F}} = -\nabla\hat{U}$ is the force operator. In free motion, or in a central field $U = U(r)$, the orbital momentum is *conserved.*

2. The Wigner distribution is usually introduced in a following way. Consider the *single-particle density matrix*

$$\rho(\mathbf{r}_1, \mathbf{r}_2) \equiv \psi(\mathbf{r}_1)\psi^*(\mathbf{r}_2). \tag{11}$$

The usual probability density is given by the diagonal (with respect to the coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$) part of (11), $\mathbf{r}_1 = \mathbf{r}_2 = \mathbf{r}$,

$$\rho(\mathbf{r}, \mathbf{r}) = |\psi(\mathbf{r})|^2. \tag{12}$$

It is convenient to introduce the center-of-mass and relative coordinates of the pair $(\mathbf{r}_1, \mathbf{r}_2)$,

$$\mathbf{R} = \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}, \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \tag{13}$$

$$\mathbf{r}_1 = \mathbf{R} + \frac{\mathbf{r}}{2}, \quad \mathbf{r}_2 = \mathbf{R} - \frac{\mathbf{r}}{2}. \tag{14}$$

Then we made the Fourier analysis with respect to the relative coordinate and introduce the momentum $\mathbf{p}$ instead of $\mathbf{r}$. This leads to the Wigner distribution

$$W(\mathbf{R},\mathbf{p}) = \int d^3r\, e^{-(i/\hbar)(\mathbf{p}\cdot\mathbf{r})}\psi(\mathbf{R}+\mathbf{r}/2)\psi^*(\mathbf{R}-\mathbf{r}/2). \tag{15}$$

/We do not need to put primes, as in the textbook, because our operators are always carrying hats, and there cannot be any confusion; here all variables are c-numbers rather than operators. Also, according to our convention, the normalizing factor $(2\pi\hbar)^{-3}$ comes together with the volume element d^3p in the momentum space./

5a. For real values of the variables $\mathbf{R}$ and $\mathbf{p}$, the complex conjugate function is

$$W^*(\mathbf{R},\mathbf{p}) = \int d^3r\, e^{(i/\hbar)(\mathbf{p}\cdot\mathbf{r})}\psi^*(\mathbf{R}-\mathbf{r}/2)\psi(\mathbf{R}+\mathbf{r}/2). \tag{16}$$

The change of integration variable $\mathbf{r}\rightarrow -\mathbf{r}$ shows that $W^* = W$, i.e. the Wigner distribution is a real-valued function (not positively defined).

5b. The integration over d^3p provides the δ-function in relative coordinate and leads to the density matrix at coinciding coordinates,

$$\int \frac{d^3p}{(2\pi\hbar)^3} W(\mathbf{R},\mathbf{p}) = \int d^3r\, \delta(\mathbf{r})\psi(\mathbf{R}+\mathbf{r}/2)\psi^*(\mathbf{R}-\mathbf{r}/2) = |\psi(\mathbf{R})|^2. \tag{17}$$

Therefore, for a normalized function, $\int d^3r\, |\psi(\mathbf{R})|^2 = 1$,

$$\langle f(\mathbf{R})\rangle \equiv \int d^3R\, f(\mathbf{R})|\psi(\mathbf{R})|^2 = \int \frac{d^3R\, d^3p}{(2\pi\hbar)^3} f(\mathbf{R})W(\mathbf{R},\mathbf{p}), \tag{18}$$

i.e. expectation values are given by the integral over the phase space as if W would be a classical distribution function (in that case it should have been positively defined).

5c. Taking in the previous equation $f(\mathbf{R}) \equiv 1$, we come, for the normalized $\psi(\mathbf{R})$, to the probabilistic normalization of the Wigner distribution,

$$\int \frac{d^3R\, d^3p}{(2\pi\hbar)^3} W(\mathbf{R},\mathbf{p}) = 1. \tag{19}$$

5d. It is clear from (12) and (18) that

$$\langle \delta(\mathbf{R}-\mathbf{R}_0)\rangle = |\psi(\mathbf{R}_0)|^2. \tag{20}$$

6a. To get an equivalent form of the Wigner distribution, we make the transformation to the wave function in the momentum representation,

$$\psi(\mathbf{R}+\mathbf{r}/2) = \int \frac{d^3p_1}{(2\pi\hbar)^3}\, e^{(i/\hbar)\mathbf{p}_1\cdot(\mathbf{R}+\mathbf{r}/2)}\phi(\mathbf{p}_1), \tag{21}$$

$$\psi^*(\mathbf{R}-\mathbf{r}/2) = \int \frac{d^3p_2}{(2\pi\hbar)^3}\, e^{-(i/\hbar)\mathbf{p}_2\cdot(\mathbf{R}-\mathbf{r}/2)}\phi^*(\mathbf{p}_2). \qquad (22)$$

Using this form in (16) we first collect the terms needed for integration over d^3r,

$$\int d^3r\, \exp[(i/\hbar)\mathbf{r}\cdot(-\mathbf{p}+\mathbf{p}_1/2+\mathbf{p}_2/2)] = (2\pi\hbar)^3\delta(\mathbf{p}-\mathbf{p}_1/2-\mathbf{p}_2/2). \quad (23)$$

Since the remaining integral contains $\exp[(i/\hbar)\mathbf{R}\cdot(\mathbf{p}_1-\mathbf{p}_2)]$, it is convenient to introduce instead of $\mathbf{p}_1$ and $\mathbf{p}_2$ new variables

$$\mathbf{p}' = \frac{1}{2}(\mathbf{p}_1+\mathbf{p}_2), \quad \mathbf{q} = \mathbf{p}_1-\mathbf{p}_2, \qquad (24)$$

or, inversely,

$$\mathbf{p}_1 = \mathbf{p}+\frac{\mathbf{q}}{2}, \quad \mathbf{p}_2 = \mathbf{p}-\frac{\mathbf{q}}{2}, \qquad (25)$$

which preserve the integration volume, $d^3p'\,d^3q = d^3p_1\,d^3p_2$, and integrate over d^3p' using $\delta(\mathbf{p}'-\mathbf{p})$ from eq. (23). This substitutes $\mathbf{p}'$ by the external momentum $\mathbf{p}$. Finally,

$$W(\mathbf{R},\mathbf{p}) = \int \frac{d^3q}{(2\pi\hbar)^3}\, e^{(i/\hbar)(\mathbf{R}\cdot\mathbf{q})}\phi(\mathbf{p}+\mathbf{q}/2)\phi^*(\mathbf{p}-\mathbf{q}/2). \qquad (26)$$

6b. The integration of eq. (26) over d^3R produces $(2\pi\hbar)^3\delta(\mathbf{q})$. Whence, we obtain the probability density in momentum space,

$$\int d^3R\, W(\mathbf{R},\mathbf{p}) = |\phi(\mathbf{p})|^2. \qquad (27)$$

The momentum functions $\phi(\mathbf{p})$ are normalized to 1 [with the volume element $d^3p/(2\pi\hbar)^3$] if the coordinate functions are normalized to 1. Therefore, for any function of momentum,

$$\langle g(\mathbf{p})\rangle = \int \frac{d^3p}{(2\pi\hbar)^3} g(\mathbf{p})|\phi(\mathbf{p})|^2 = \int \frac{d^3R\,d^3p}{(2\pi\hbar)^3} g(\mathbf{p})W(\mathbf{R},\mathbf{p}). \qquad (28)$$

Indeed, the Wigner distribution plays the role similar to the *probability density in phase space* and gives the formulation of quantum mechanics formally close to classical mechanics.

3. The definitions: a *transpose* operator $\hat{F}^T$,

$$\langle n|\hat{F}^T|m\rangle = \langle m|\hat{F}|n\rangle; \qquad (29)$$

a *complex conjugate* operator $\hat{F}^*$,

$$\langle n|\hat{F}^*|m\rangle = \langle n|F|m\rangle^*; \qquad (30)$$

a *Hermitian conjugate* operator $\hat{F}^\dagger$,

$$\langle n|\hat{F}^\dagger|m\rangle = \langle m|\hat{F}|n\rangle^*, \tag{31}$$

which means

$$\hat{F}^\dagger = (\hat{F}^T)^*; \tag{32}$$

an *inverse* operator $\hat{F}^{-1}$,

$$\hat{F}\hat{F}^{-1} = \hat{F}^{-1}\hat{F} = \hat{1} \text{ (unit operator)}. \tag{33}$$

First three operators are real,

$$\hat{\mathcal{P}}^* = \hat{\mathcal{P}}, \quad \hat{\mathcal{D}}(a)^* = \hat{\mathcal{D}}(a), \quad \hat{\mathcal{M}}^*(\alpha) = \hat{\mathcal{M}}(\alpha); \tag{34}$$

the operator $\hat{k} = \hat{p}/\hbar$ is imaginary,

$$\hat{k}^* = i\frac{d}{dx} = -\hat{k}. \tag{35}$$

For real operators, transpose and Hermitian conjugation coincide. Since

$$\langle n|\hat{\mathcal{P}}|m\rangle = \int dx\, \psi_n^*(x)\mathcal{P}\psi_m(x) = \int dx\, \psi_n^*(x)\psi_m(-x) =$$

$$\int dx\psi_n^*(-x)\psi_m(x) = \int dx\, (\hat{\mathcal{P}}\psi_n(x))^*\psi_m(x), \tag{36}$$

the inversion operator is Hermitian,

$$\hat{\mathcal{P}}^\dagger = \hat{\mathcal{P}}^T = \hat{\mathcal{P}}. \tag{37}$$

For the *displacement* operator we find

$$\langle n|\hat{\mathcal{D}}(a)|m\rangle = \int dx\, \psi_n^*(x)\psi_m(x-a) =$$

$$\int dx\, \psi_n^*(x+a)\psi_m(x) = \int dx\, (\hat{\mathcal{D}}(-a)\psi_n(x))^*\psi_m(x), \tag{38}$$

which means

$$\hat{\mathcal{D}}^\dagger(a) = \hat{\mathcal{D}}^T(a) = \hat{\mathcal{D}}(-a). \tag{39}$$

For the *scaling* operator,

$$\langle n|\hat{\mathcal{M}}(\alpha)|m\rangle = \int dx\, \psi_n^*(x)\sqrt{\alpha}\psi_m(\alpha x). \tag{40}$$

Changing variables $y = \alpha x$ and renaming back $y \to x$, we obtain

$$\langle n|\hat{\mathcal{M}}(\alpha)|m\rangle = \frac{1}{\sqrt{\alpha}}\int dx\, \psi_n(x/\alpha)\psi_m(x) = \int dx\, (\hat{\mathcal{M}}(\alpha^{-1})\psi_n(x))^*\psi_m(x). \tag{41}$$

Thus,

$$\hat{\mathcal{M}}^\dagger(\alpha) = \hat{\mathcal{M}}^T(\alpha) = \hat{\mathcal{M}}(1/\alpha). \tag{42}$$

The first three operators cannot have eigenfunctions (not identically equal to zero) which would correspond to the eigenvalue 0; therefore for these operators the inverse operator is well defined,

$$\hat{\mathcal{P}}^{-1} = \hat{\mathcal{P}}, \quad \hat{\mathcal{D}}(a)^{-1} = \hat{\mathcal{D}}(-a), \quad \hat{\mathcal{M}}(\alpha)^{-1} = \hat{\mathcal{M}}(1/\alpha). \tag{43}$$

In all cases we assume that the wave functions are *square integrable*, $\int dx|\psi(x)|^2 < \infty$. This is especially important for the operator $\hat{k}$. Since it is imaginary, $\hat{k}^\dagger = -\hat{k}^T$. But it is Hermitian on a class of square integrable functions (we have demonstrated this for the momentum operator $\hat{p} = \hbar\hat{k}$),

$$\hat{k}^\dagger = -\hat{k}^T = \hat{k}. \tag{44}$$

The inverse operator for the operator $\hat{k}$ does not exist since, for any $\psi(x)$, the primitive function $i\int dx\,\psi(x)$ which should give back $\psi(x)$ after the action by $-i(d/dx)$ is defined only up to a constant. The reason is that the constant is an eigenfunction of the operator $\hat{k}$ corresponding to the eigenvalue 0 which precludes the unique definition of the inverse operator.

4. The general solution of the Schrödinger equation for free motion with the initial condition $\Psi(x, t = 0) = \psi(x)$ is given by the independent propagation of plane waves with momentum p and energy $\epsilon(p) = p^2/2m$,

$$\Psi(x,t) = \int \frac{dp}{2\pi\hbar}\, e^{(i/\hbar)[px-(p^2/2m)t]}\phi(p), \tag{45}$$

where $\phi(p)$ is the probability amplitude to have momentum p in the initial wave function $\psi(x)$, i.e. Fourier expansion of $\psi(x)$,

$$\phi(p) = \int dx'\, e^{-(i/\hbar)px'}\psi(x'). \tag{46}$$

Therefore

$$\Psi(x,t) = \int \frac{dx'\,dp}{2\pi\hbar} e^{(i/\hbar)[p(x-x')-(p^2/2m)t]}\psi(x'), \tag{47}$$

or, since the initial point can be arbitrarily taken at $t = t'$ instead of $t = 0$ as in eq. (47),

$$\Psi(x,t) = \int \frac{dx'\,dp}{2\pi\hbar} e^{(i/\hbar)[p(x-x')-(p^2/2m)(t-t')]}\Psi(x',t'). \tag{48}$$

This allows us to determine the Green function

$$G(x,t;x',t') = \int \frac{dp}{2\pi\hbar} e^{(i/\hbar)[p(x-x')-(p^2/2m)(t-t')]}. \tag{49}$$

This is a particular case of the general result valid for any time-independent Hamiltonian $\hat{H}$ with the spectrum $\{E_n\}$ and corresponding stationary eigenfunctions $\psi_n(x)$,

$$\hat{H}\psi_n = E_n\psi_n. \tag{50}$$

The Green function for the general situation is

$$G(x,t;x',t') = \sum_n \psi_n(x)\psi_n^*(x')e^{-(i/\hbar)E_n(t-t')}. \tag{51}$$

In our case the sum over the spectrum becomes the integral $\int dp/(2\pi\hbar)$, the eigenfunctions are $\psi_p(x) = \exp[(i/\hbar)px]$, and energies $E_n \to \epsilon(p)$. The standard calculation of the Gaussian integral in (49) gives

$$G(x,t;x',t') = \sqrt{\frac{m}{2i\pi\hbar(t-t')}}\exp\left[\frac{im(x-x')^2}{2\hbar(t-t')}\right], \tag{52}$$

with the obvious generalization for the three-dimensional case,

$$G(\mathbf{r},t;\mathbf{r}',t') = \left[\frac{m}{2i\pi\hbar(t-t')}\right]^{3/2}\exp\left[\frac{im(\mathbf{r}-\mathbf{r}')^2}{2\hbar(t-t')}\right]. \tag{53}$$

The effective propagation corresponds to the region where the exponent is not very big (to avoid wild oscillations and compensation), $|x-x'| \sim [\hbar(t-t')/m]^{1/2}$, in accordance with the previous estimates of the quantum spreading.

5. The Hamiltonian of the problem is

$$\hat{H} = \frac{\hat{p}^2}{2m} - f\hat{x}, \quad f = e\mathcal{E}. \tag{54}$$

a. The Ehrenfest equations of motion can be derived by the straightforward calculations of the commutators, or just by the analogy to classical mechanics,

$$\frac{d\langle\hat{x}\rangle}{dt} = \frac{\langle\hat{p}\rangle}{m}, \tag{55}$$

$$\frac{d\langle\hat{p}\rangle}{dt} = f. \tag{56}$$

The time integration leads to

$$\langle\hat{p}\rangle = \langle\hat{p}\rangle_0 + ft, \tag{57}$$

$$\langle\hat{x}\rangle = \langle\hat{x}\rangle_0 + \frac{\langle\hat{p}\rangle_0}{m}t + \frac{f}{2m}t^2. \tag{58}$$

A semiclassical meaning of these expressions is evident.

b. In the coordinate representation $\hat{x} = x$, $\hat{p} = -i\hbar(d/dx)$, and the wave equation for the stationary state with energy E is

$$-\frac{\hbar^2}{2m}\psi_E(x) - fx\psi_E(x) = E\psi_E(x), \tag{59}$$

whereas in the momentum representation $\hat{x} = i\hbar(d/dp)$, $\hat{p} = p$, and the equation contains only the first derivative,

$$\frac{p^2}{2m}\,\phi_E(p) - i\hbar f\frac{d}{dp}\phi_E(p) = E\phi_E(p). \tag{60}$$

Of course, it is sufficient to solve only one of those equations; then it is possible to obtain the remaining counterpart by the Fourier transformation.

The momentum representation (60) allows one to integrate the equation directly and obtain

$$\phi_E(p) = a(E)\exp\left[\frac{i}{\hbar}\left(\frac{Ep}{f} - \frac{p^3}{6m\hbar f}\right)\right]. \tag{61}$$

The much more complicated coordinate functions are the so-called Airy functions which can be expressed in terms of cylindrical functions of order 1/3. Any value of energy E from $-\infty$ to $+\infty$ is possible as seen from the form of the potential energy $U = -fx$ which allows only infinite motion and continuous quantum spectrum. All solutions are not degenerate because the potential allows only the motion from one side, at $f > 0$ from $-\infty$ to the turning point and back. Therefore each eigenfunction is fully characterized by its energy E.

c. The *orthogonality* of functions for $E \neq E'$ is seen from

$$\int \frac{dp}{2\pi\hbar}\,\phi^*_{E'}(p)\phi_E(p) = a^*(E')a(E)\int \frac{dp}{2\pi\hbar}\,e^{(i/\hbar f)p(E-E')} = |a(E)|^2 f\delta(E-E'). \tag{62}$$

The convenient choice of the normalization [to $\delta(E - E')$] is

$$a(E) = \frac{1}{\sqrt{f}}. \tag{63}$$

The *completeness* of the set of the eigenfunctions in general is expressed as

$$\sum_n \psi_n(x)\psi^*_n(x') = \delta(x, x'). \tag{64}$$

In our case the summation index n is to be substituted by the continuous integration variable E,

$$\int_{-\infty}^{\infty} dE\,\phi_E(p)\phi^*_E(p') = \frac{1}{f}e^{(i/6\hbar mf)(p'^3-p^3)}\int dE\,e^{(iE/\hbar f)(p-p')}. \tag{65}$$

The integral in the last expression of (65) equals $2\pi f\hbar\delta(p-p')$. At $p=p'$ the exponents in front of the integral cancel, and the result is

$$\int_{-\infty}^{\infty} dE\,\phi_E(p)\phi_E^*(p') = 2\pi\hbar\delta(p-p'), \tag{66}$$

as it should be with our convention of the momentum integration $\int dp/(2\pi\hbar)$.

d. According to the general expression (51), which is valid in an arbitrary representation,

$$G(p,t;p',t') = \int dE\,\phi_E(p)\phi_E^*(p')e^{-(i/\hbar)E(t-t')}. \tag{67}$$

With the explicit form of our wave functions,

$$G(p,t;p',t') = 2\pi\hbar\delta(p-p'-f(t-t'))e^{-(i/6\hbar mf)(p^3-p'^3)}. \tag{68}$$

As a check, we see that at the initial moment $t=t'$

$$G(p,t;p',t) = 2\pi\hbar\delta(p-p'). \tag{69}$$

The delta-function in (68) corresponds to the particle acceleration by the electric field, see eq. (57). The phase factor comes from the energy increase due to the acceleration, $dp/dt=f$,

$$\int dt\,\frac{p^2}{2m} = \int dp\,\frac{p^2}{2m}\,\frac{dt}{dp} = \frac{p^3}{6mf}. \tag{70}$$