Problem Set 5: Aharonov-Bohm, Propagators & Coherent States
Graduate Quantum I
Physics 6572

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Due Friday Sept. 26

Last correction at September 15, 2014, 9:59 pm

Potentially useful reading

Sakurai and Napolitano, sections 2.3 (coherent states), 2.6 (path integrals), 3.4 (density matrices)

Schumacher & Westmoreland section 13.3 (coherent states)

Weinberg section 3.2 (delta functions), section 9.6 (Greens functions)

P.W. Anderson, "Basic Notions of Condensed Matter Physics", section 3E p. 107-113 (advanced Green's functions)

5.1 **Dirac δ-functions.** (Math) ③

Quantum bound-state wavefunctions are unit vectors in a complex Hilbert space. If there are N particles in 3 dimensions, the Hilbert space is the space of complex-valued functions $\psi(\mathbf{x})$ with $\mathbf{x} \in \mathbb{R}^{3N}$ whose absolute squares are integrable: $\int \mathrm{d}\mathbf{x} |\psi(\mathbf{x})|^2 < \infty$.

But what about unbound states? For example, the propagating plane-wave states $\psi(x) = |k\rangle \propto \exp(-\mathrm{i}kx)$ for a free particle in one dimension? Because unbound states are spread out over an infinite volume, their probability density at any given point is zero – but we surely don't want to normalize $|k\rangle$ by multiplying it by zero.

Mathematicians incorporate continuum states by extending the space into a *rigged Hilbert space*. The trick is that the unbound states form a *continuum*, rather than a discrete spectrum – so instead of summing over states to decompose wavefunctions $|\phi\rangle = \mathbb{1}\phi = \sum_n |n\rangle\langle n|\phi\rangle$ we integrate over states $\phi = \mathbb{1}\phi = \int \mathrm{d}k\, |k\rangle\langle k|\phi\rangle$. This tells us how we must normalize our continuum wavefunctions: instead of the Kronecker-δ function $\langle m|n\rangle = \delta_{mn}$ enforcing orthonormal states, we demand $|k'\rangle = \mathbb{1}|k'\rangle = \int \mathrm{d}k\, |k\rangle\langle k|k'\rangle = |k'\rangle = \int \mathrm{d}k\, |k\rangle \delta(k-k')$ telling us that $\langle k|k'\rangle = \delta(k-k')$ is needed to ensure the useful decomposition $\mathbb{1} = \int \mathrm{d}k\, |k\rangle\langle k|$.

Let's work out how this works as physicists, by starting with the particles in a box, and then taking the box size to infinity. For convenience, let us work in a one dimensional box $-L/2 \le x < L/2$, and use *periodic boundary conditions*, so $\psi(-L/2) = \psi(L/2)$ and $\psi'(-L/2) = \psi'(L/2)$. This choice allows us to continue to work with plane-wave states $|n\rangle \propto \exp(-\mathrm{i}k_n x)$ in the box. (We could have used a square well with infinite sides, but then we'd need to fiddle with wave-functions $\propto \sin(kx)$.)

(a) What values of k_n are allowed by the periodic boundary conditions? What is the separation Δk between successive wavevectors? Does it go to zero as $L \to \infty$, leading to a continuum of states?

To figure out how to normalize our continuum wavefunctions, we now start with the relation $\langle m|n\rangle = \delta_{mn}$ and take the continuum limit. We want the normalization N_k of the continuum wavefunctions to give $\int_{-\infty}^{\infty} N_k N_{k'} \exp(-\mathrm{i}(k'-k)x)\mathrm{d}x = \delta(k'-k)$.

(b) What is the normalization $\langle x|n\rangle = N_n \exp(\mathrm{i}k_n x)$ for the discrete wave-functions in the periodic box, to make $\langle m|n\rangle = \int_{-L/2}^{L/2} N_n N_m \exp(-\mathrm{i}(k_m - k_n)x)\mathrm{d}x = \delta_{mn}$? Write $\mathbb{1} = \sum_n |n\rangle\langle n|$, and change the sum to an integral in the usual way ($\int \mathrm{d}k\, |k\rangle\langle k| \approx \sum_n \Delta k\, |n\rangle\langle n|$). Show that the normalization of the continuum wavefunctions must be $N_k = 1/\sqrt{2\pi}$, so $\psi_k(x) = \langle x|k\rangle = \exp(\mathrm{i}kx)/\sqrt{2\pi}$. (Hint: If working with operators is confusing, ensure that $\langle x|\mathbb{1}|x'\rangle$ for $-L/2 < x, x' < L/2$ is the same for $\mathbb{1} = \sum_n |n\rangle\langle n|$ (valid in the periodic box) and for $\mathbb{1} = \int \mathrm{d}k|k\rangle\langle k|$ (valid for all x).

Notice some interesting ramifications:

I. The fact that our continuum plane waves have normalization $1/\sqrt{2\pi}$ incidentally tells us one form of the δ function:

$$\delta(k'-k) = \langle k|k'\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-\mathrm{i}(k'-k)x}\mathrm{d}x. \tag{1}$$

Also, $\delta(x'-x) = 1/(2\pi)\int_{-\infty}^{\infty} \mathrm{d}k \exp(\mathrm{i}k(x'-x))$.

II. The same normalization is used for 'position eigenstates' $|x\rangle$, so $\langle x'|x\rangle = \delta(x'-x)$ and $\mathbb{1} = \int \mathrm{d}x|x\rangle\langle x|$.

III. The Fourier transform can be viewed as a change of variables from the basis $|x\rangle$ to the basis $|k\rangle$:

$$\begin{aligned}\widetilde{\phi}(k) &= \langle k|\phi\rangle = \langle k|\mathbb{1}|\phi\rangle \\ &= \int \mathrm{d}x\langle k|x\rangle\langle x|\phi\rangle \\ &= 1/\sqrt{2\pi}\int \mathrm{d}x \exp(-\mathrm{i}kx)\phi(x)\end{aligned} \tag{2}$$

Note that this definition is different from that I used in the appendix of my book (Statistical Mechanics: Entropy, Order Parameters, and Complexity, http://pages.physics.cornell.edu/~sethna/Stat Mech/EntropyOrderParametersComplexity.pdf); there the 2π is placed entirely on the inverse Fourier transform, which here it is split symmetrically between the two, so the inverse Fourier transform is

$$\phi(x) = \langle x|\phi\rangle = \langle x|\mathbb{1}|\phi\rangle \tag{3}$$

$$= \int \mathrm{d}k\langle x|k\rangle\langle k|\phi\rangle \tag{4}$$

$$= 1/\sqrt{2\pi}\int \mathrm{d}k \exp(\mathrm{i}kx)\widetilde{\phi}(k).$$

IV. The Dirac δ-function can be written in many different ways. It is basically the limit[1] as $\epsilon \to 0$ of sharply-peaked, integral-one functions of width ϵ and height $1/\epsilon$ centered at zero. Let's use this to derive the useful relation:

$$\lim_{\epsilon\to 0+} \frac{1}{x - \mathrm{i}\epsilon} = p.v.\frac{1}{x} + \mathrm{i}\pi\delta(x). \tag{5}$$

Here all these expressions are meant to be inside integrals, and p.v. is the Cauchy principal value of the integral:[2]

$$p.v. \int_{-\infty}^{\infty} = \lim_{\epsilon\to 0+} \int_{-\infty}^{-\epsilon} + \int_{\epsilon}^{\infty} . \tag{6}$$

(c) Note that $\epsilon/(x^2+\epsilon^2)$ has half-width ϵ at half-maximum, height ϵ, and integrates to π, so basically (i.e., in the weak limit) $\lim_{\epsilon\to 0} \epsilon/(x^2+\epsilon^2) = \pi\delta(x)$. Argue that $\lim_{\epsilon\to 0} \int f(x)/(x-\mathrm{i}\epsilon)\mathrm{d}x = p.v. \int f(x)/x\,\mathrm{d}x + \mathrm{i}\pi f(0)$. (Hints: The integral of $1/(1+y^2)$ is $\arctan(y)$, which becomes $\pm\pi/2$ at $y = \pm\infty$. Multiply numerator and denominator by $x + \mathrm{i}\epsilon$.)

5.2 **Momentum Space Propagator.** (Sakurai Exercise 2.33) ②

As given in Eq.(2.6.26) in Sakurai, the propagator in position space is

$$\begin{aligned} K(\mathbf{x}'', t; \mathbf{x}', t_0) &= \textstyle\sum_{a'} \langle \mathbf{x}''|a'\rangle\langle a'|\mathbf{x}'\rangle \exp\left[\frac{-\mathrm{i}E_{a'}(t-t_0)}{\hbar}\right] \\ &= \textstyle\sum_{a'} \langle \mathbf{x}''| \exp\left(\frac{-\mathrm{i}Ht}{\hbar}\right)|a'\rangle\langle a'| \exp\left(\frac{\mathrm{i}Ht_0}{\hbar}\right)|\mathbf{x}'\rangle \end{aligned}$$

The analogous propagator in momentum space is given by $\langle \mathbf{p}'', t|\mathbf{p}', t_0\rangle$. *Derive an explicit expression for $\langle \mathbf{p}'', t|\mathbf{p}', t_0\rangle$ for the free particle case.*

5.3 **Harmonic oscillator spectrum: The propagator.** (Path integrals) ③

(a) *Show that the trace of the propagator can be written in terms of the energy eigenvalues:*

$$\int_{-\infty}^{\infty} K(x, t_2; x, t_1)\mathrm{d}x = \sum_n \exp(-\mathrm{i}E_n(t_2 - t_1)/\hbar). \tag{7}$$

(Hint: write

$$\begin{aligned} K &= \langle x_2|U(t_2 - t_1)|x_1\rangle = \langle x_2|\mathrm{e}^{-\mathrm{i}H(t_2-t_1)/\hbar}|x_1\rangle \\ &= \langle x_2|\mathbb{1}\mathrm{e}^{-\mathrm{i}H(t_2-t_1)/\hbar}|x_1\rangle \end{aligned}$$

[1] Clearly this is not a limit in the ordinary sense: the difference between functions does not go to zero as ϵ goes to zero, but rather (within ϵ of the origin) has large positive and negative values that cancel. It is a *weak limit* – when integrated against any smooth functions, the differences go to zero.

[2] If $f(x)$ is positive at zero, $\int f(x)/x\,\mathrm{d}x$ is the sum of minus infinity for $x < 0$ and positive infinity for $x > 0$; taking the principal value tells us to find the sum of these two canceling infinities by chopping them symmetrically about zero.

and insert a complete set of energy eigenstates for $\mathbb{1}$.)

(b) *Sum the geometrical series in eqn 7 for a one-dimensional harmonic oscillator of frequency ω.*

The propagator for the harmonic oscillator is

$$K_{HO}(x_2, t_2; x_1, t_1) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega(t_2 - t_1))}} \exp\left[\frac{im\omega}{2\hbar \sin(\omega(t_2 - t_1))}\{(x_2^2 + x_1^2)\cos(\omega(t_2 - t_1)) - 2x_2x_1)\right].$$

(There is a typo in Sakurai's formula 2.6.18).

(c) *Write $K_{HO}(x, t_2, x, t_1) = f(t)\exp(-iA(t)x^2)$. Evaluate the trace. Show that you get the same answer as part (b).* (Hint: Use the Gaussian integral formula $\int_{-\infty}^{\infty} \exp(-iA(t)x^2) = \sqrt{\pi/(iA)}$. You may want to use the half-angle formula $\sin(a/2) = \sqrt{1/2(1 - \cos(a)}$.)

5.4 **Aharonov-Bohm Wire.** (ParallelTransport) ③

What happens to the electronic states in a thin metal loop as a magnetic flux Φ_B is threaded through it? This was a big topic in the mid-1980's, with experiments suggesting that the loops would develop a spontaneous current, that depended on the flux Φ_B/Φ_0, with $\Phi_0 = hc/e$ the 'quantum of flux' familiar from the Bohm-Aharnov effect. In particular, Nandini Trivedi worked on the question while she was a graduate student here:

> Nandini Trivedi and Dana Browne, 'Mesoscopic ring in a magnetic field: Reactive and dissipative response', *Phys. Rev. B* **38**, 9581-9593 (1988);

she's now a faculty member at Ohio State.

Some of the experiments clearly indicated that the periodicity in the current went as $\Phi_0/2 = hc/2e$ – half the period demanded by Bohm and Aharonov from fundamental principles. (This is OK; having a *greater* period would cause one to wonder about fractional charges.) Others found (noisier) periods of Φ_0. Can we do a free-particle-on-a-ring calculation to see if for some reason we get half the period too?

Consider a thin wire loop of radius R along $x^2 + y^2 = R^2$. Let a solenoid containing magnetic flux Φ_B, thin compared to R, lie along the $\hat{z}$ axis, with effectively no magnetic field outside the solenoid. Let ϕ be the angle around the circle with respect to the positive x-axis. (Don't confuse the flux Φ_B with the angle ϕ!) We'll assume the wire confines the electron to lie along the circle, so we're solving a one-dimensional Schrödinger's equation along the coordinate $s = R\phi$ around the circle. Assume the electrons experience an arbitrary potential $V(s)$ along the circumference $C = 2\pi R$ of the wire loop.[3]

[3]You may imagine this potential as due to random imperfections or impurities in the wire loop.

(a) *If $\vec{\mathbf{A}} = a(r)\hat{\phi}$, what is the value of $a(R)$ for a solenoid flux Φ_B?*

(b) *Using this $\vec{\mathbf{A}}$ field, write the one-dimensional time-independent Schrödinger equation giving the eigenenergies for electrons on this ring. What is the boundary conditions for the electron wavefunction ψ at $s = 0$ and $s = C$?* (Hint: the wire is a circle; no parallel transport yet. I'm not asking you to solve the equation – only to write it down.)

Deriving the Bohm-Aharonov effect using Schrödinger's equation is easiest done using a singular gauge transformation.[4]

(c) *Consider the gauge transformation $\Lambda(r, \phi) = -\phi\Phi_B/(2\pi)$. Show that $\vec{\mathbf{A}}' = \vec{\mathbf{A}} + \nabla\Lambda$ is zero along the wire for $0 < s < C$, so that we are left with a zero-field Schrödinger equation. What happens at the endpoint C? What is the new boundary condition for the electron wave function ψ' after this gauge transformation? Does the effect vanish for $\Phi_B = n\Phi_0$ for integer n, as the Bohm-Aharonov effect says it should?*

Realistically, the electrons in a large, room-temperature wire get scattered by phonons or electron-hole pairs (effectively, a quantum measurement of sorts) long before they propagate around the whole wire, so these effects were only seen experimentally when the wires were cold (to reduce phonons and electron-hole pairs) and 'mesoscopic' (tiny, so the scattering length is comparable to or larger than the circumference).

Finally, let's assume free electrons, so $V(s) = 0$. What's more, to make things simpler, let's imagine that there is only one electron in the wire.

(d) *Ignoring the energy needed to confine the electrons into the thin wire, solve the one-dimensional Schrödinger equation to give the ground state of the electron as a function of Φ_B. Plot the current*[5] *in the wire as a function of Φ_B. Is it periodic with period Φ_0, or periodic with period $\Phi_0/2$?*

In the end, it was determined that there were two classes of experiments. Those that measured many rings at once (measuring an average current, an easier experiment) got periodicity of $hc/2e$, while those that attempted the challenge of measuring one mesoscopic ring at a time find hc/e.

5.5 **Evolving Schrödinger: Coherent states.** (Computation) ③

In this exercise, we shall build upon the numerical work of exercise 3.6 (free particle evolution), exercise 4.2 (Baker-Campbell Hausdorff idenity), and exercise 4.3 (Coherent States). We shall solve the time-dependent Schrödinger equation for a harmonic oscillator in its ground state, and after the ground state is translated to the side by a distance x_0.

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[4]You could just solve the original Schrödinger equation. But by doing the singular gauge transformation, you are left with a familiar Schrödinger equation without an $\vec{\mathbf{A}}$ field, albeit with a funny boundary condition.

[5]This is the probability current $\mathbf{J}$. In the absence of a field, $\mathbf{J} = (\hbar/(2mi)(\psi^*\nabla\psi - \psi\nabla\psi^*)$. (If you don't already recognize this formula, look up the derivation!) Since the probability current is a physical quantity, it must be gauge invariant, so you can use this same formula in the singular gauge to estimate the current.

The time-dependent Schrödinger equation for our one-dimensional quantum system is:

$$\begin{aligned}
\mathrm{i}\hbar\frac{\partial\psi}{\partial t} &= -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi = H\psi = H_{\mathrm{kin}}\psi + H_{\mathrm{pot}}\psi \\
\psi(t) &= U(t)\psi(0) = \mathrm{e}^{-\mathrm{i}Ht/\hbar}\psi(0) = \mathrm{e}^{-\mathrm{i}H_{\mathrm{kin}}t/\hbar - \mathrm{i}H_{\mathrm{pot}}t/\hbar}\psi(0)
\end{aligned} \tag{8}$$

As in the last exercise, we use the constants for McEuen's bouncing buckyballs, with $m = 60m_C \sim 12 * 60m_p$ and the frequency to $\omega = 10^{12}$ radians/sec, and will evaluate it at $N_p = 200$ points spanning $L = 30a_0$,

In the free particle example (no potential energy), we advanced time by dt by multiplying the Fourier transform by $U_{\mathrm{kin}}(k, dt) = \exp(\mathrm{i}(\hbar^2k^2/2m)dt/\hbar)$. If, on the other hand, there were no *kinetic* energy (infinite mass), we could solve for the time evolution $\psi(x,t) = U_{\mathrm{pot}}(t)\psi(x, t = 0)$ by multiplying $\psi(x)$ in real space by a time-dependent phase depending on position:

$$\begin{aligned}
\psi(x, t + dt) &= U_{\mathrm{pot}}(dt)\psi(x,t) = \mathrm{e}^{-\mathrm{i}H_{\mathrm{pot}}dt/\hbar}\psi(x,t) \\
&= \mathrm{e}^{-\mathrm{i}V(x)dt/\hbar}\psi(x,t).
\end{aligned} \tag{9}$$

To approximately solve Schrödinger's time evolution, we alternate advancing the wave function in real space and Fourier space, using the Baker–Campbell–Hausdorff formula of exercise 4.2(b):

$$\psi(t + dt) = \mathrm{e}^{-\mathrm{i}H_{\mathrm{kin}}t/\hbar - \mathrm{i}H_{\mathrm{pot}}t/\hbar}\psi(0) \quad \approx \mathrm{e}^{-\mathrm{i}H_{\mathrm{pot}}t/2\hbar}\mathrm{e}^{-\mathrm{i}H_{\mathrm{kin}}t/\hbar}\mathrm{e}^{-\mathrm{i}H_{\mathrm{pot}}t/2\hbar}\psi(0) = U_{\mathrm{pot}} \tag{10}$$

(a) *Define the two arrays* UkinTildeDt *and* UpotDtOver2. *Define the initial wavefunction $\psi[0](x)$.* (Hint: If your implementation stores $\psi[n][x]$ as a two-dimensional complex array, you may want to allocate it and initialize $\psi[0][x]$ as part of that array.)

(b) *Evolve the wavefunction to a time equal to twice the period P of the oscillator, in steps of $dt = P/100$, storing your answer after each step. Plot $\psi(x, P/5)$, showing the real part, the imaginary part, and the absolute value all on the same graph.* (Why don't we plot $|\psi^2(x)|$ on this graph?) *If possible, animate these three curves; otherwise, plot several snapshots until you see the evolution. What happens to the probability density? Why? What happens to the real and imaginary parts? Why?*

(c) *Now shift the wavefunction $\psi(x, t = 0) = \psi_0(x - x0)$, with $x_0 = 10a_0$, where a_0 is the root-mean-square width of the ground state wavefuction (see exercise 3.6). Time evolve as in part (b). How does the evolution compare to a classical particle in the harmonic well?*

(d) *Using your answer to exercise 4.3(d), write the initial wavefunction for part (c) in terms of a coherent state. What is λ?*

For photons and phonons and other harmonic systems, the coherent states evolve just as classical particles would.

5.6 **Coherent State Evolution.** (Operator algebra) ③

Consider the annihilation operator a for a simple harmonic oscillator, transformed into the time-dependent Heisenberg-representation operator $\mathbf{a}_{\mathrm{H}}(t)$:

$$\mathbf{a}_{\mathrm{H}}(t) = \mathrm{e}^{\mathrm{i}\mathcal{H}t/\hbar} a \mathrm{e}^{-\mathrm{i}\mathcal{H}t/\hbar} = U^{\dagger}(t) a U(t). \tag{11}$$

The time evolution for an operator in the Heisenberg representation is given by the commutator with the Hamiltonian, so

$$\frac{\mathrm{d}\mathbf{a}_{\mathrm{H}}}{\mathrm{d}t} = \frac{\mathrm{i}\mathcal{H}}{\hbar}\mathbf{a}_{\mathrm{H}} - \mathbf{a}_{\mathrm{H}}\frac{\mathrm{i}\mathcal{H}}{\hbar} = -\mathrm{i}/\hbar[\mathbf{a}_{\mathrm{H}}, \mathcal{H}]. \tag{12}$$

You may use the fact that the Hamiltonian for the harmonic oscillator in the Schrödinger representation is $\mathcal{H} = \hbar\omega(a^{\dagger}a + \frac{1}{2})$, and that $[a, a^{\dagger}] = 1$.

(a) *Calculate* $[\mathbf{a}_{\mathrm{H}}, \mathcal{H}]$*, and write it in terms of* $\mathbf{a}_{\mathrm{H}}$*. What is* $\mathrm{d}\mathbf{a}_{\mathrm{H}}/\mathrm{d}t$*?* (Simplify your answers until they only involve $\mathbf{a}_{\mathrm{H}}$ and constants, not $\mathcal{H}$ or a.)

(b) *Show that* $\mathbf{a}_{\mathrm{H}}(t) = \exp(-\mathrm{i}\omega t)\mathbf{a}_{\mathrm{H}}(0) = \exp(-\mathrm{i}\omega t)a$ *is the solution to the time evolution you found in part (a).* (Hint: This can also be a check for part (a).)

We discovered in exercise 5 that the probability density for a displaced harmonic oscillator ground state oscillates like a classical particle with the oscillator frequency ω. In another exercise, we showed that a displaced harmonic oscillator ground state is one example of a *coherent state*, an eigenstate of the annihilation operator a:

$$a|\lambda\rangle = \lambda|\lambda\rangle, \tag{13}$$

which is also normalized $\langle\lambda|\lambda\rangle = 1$. Here $\lambda \in \mathbb{C}$ can be any complex number.

(c) *In the Schrödinger representation*[6] *show that a coherent state* $|\lambda\rangle$ *evolves after a time* t *to a state* $|\xi\rangle = U(t)|\lambda\rangle$ *which is also an eigenstate of the annihilation operator* a*. What is its eigenvalue* $\tilde{\lambda}$*?* (Hints: Multiply $a|\xi\rangle = aU(t)|\lambda\rangle$ on the left by $\mathbb{1} = U(t)U(-t)$ and use part (b). You don't need to *compute* $U(t)|\lambda\rangle$, you just need to show it is an eigenstate of a.)

Since there is only one coherent state with eigenvalue $\tilde{\lambda}$, our evolved state $U(t)|\lambda\rangle = C|\tilde{\lambda}\rangle$ for some constant C. Since time evolution conserves probability (and hence $U(t)$ is unitary), $\langle\lambda|U^{\dagger}(t)U(t)|\lambda\rangle = |C|^2 = 1$, so C is a pure phase.

It so happens that, for the standard definition of coherent states, the phase C is independent of λ, but depends on time.

(d) *Calculate* $C(t)$ *for the special case* $\lambda = 0$. (Hint: the coherent state with $\lambda = 0$ is the ground state of the harmonic oscillator. You don't need to know the solutions of previous sections to solve this.)

[6] As opposed to the Heisenberg representation of part (b).