**Problem Set 5: Miscellaneous**
**Graduate Quantum I**
**Physics 6572**
James Sethna
Due Monday Oct 29
Last correction at October 29, 2012, 2:51 pm

**Reading**
Sakurai and Napolitano, chapter 4 and 7 (chapter 6, Sakurai red 'Revised' edition)

5.1 **A peculiar unitary matrix.** *Sakurai & Napolitano, problem 3.3, "Consider the $2 \times 2$ matrix defined by. . . "* (This is problem 3.2 in the older red 'Revised edition'.) (Hint: part (a) can be done without writing out the components. For part (b), I first did it in Mathematica, and then figured out that one can find the answer by rotating the coordinate system until $\mathbf{a} \propto \hat{z}$.)

5.2 **Spin-1 Hamiltonian.** *Sakurai & Napolitano, problem 4.12, red version also 4.12, "The Hamiltonian for a spin 1 system. . . ".* Omit the questions about time-reversal invariance. (Hint: I needed to construct $S_y$ and $S_z$ from $J_{\pm}$.)

5.3 **Harmonic Fermi Sea.** *Sakurai & Napolitano, problem 7.2, red version 6.1, "N identical spin ½ . . . "*

5.4 **Identical spin-1 addition.** *Sakurai & Napolitano, problem 7.3, red version 6.2, "It is obvious. . . "*

5.5 **Triangle of spinless bosons.** *Sakurai & Napolitano, problem 7.5, red version 6.4, "Three spin 0 particles. . . "*

5.6 **Anticommutation and number.** (Corrected version of Sakurai & Napolitano, problem 7.7.) *Show that, for an operator a that, with its adjoint, obeys the anticommutation relations $\{a, a\} = \{a^{\dagger}, a^{\dagger}\} = 0$ and $\{a, a^{\dagger}\} = aa^{\dagger} + a^{\dagger}a = 1$, that the operator $N = a^{\dagger}a$ only has eigenstates with the eigenvalues 0 and 1.*

5.7 **Lithium ground state symmetry.** (Quantum) ③

A simple model for heavier atoms, that's surprisingly useful, is to ignore the interactions between electrons (the *independent electron* approximation).[1]

$$\mathcal{H}^{Z} = \sum_{i=1}^{Z} p_i^2/2m - k_{\varepsilon}Ze^2/r_i \qquad (1)$$

---

[1]Here $k_{\varepsilon} = 1$ in CGS units, and $k_{\varepsilon} = 1/(4\pi\varepsilon_0)$ in SI units. We are ignoring the slight shift in effective masses due to the motion of the nucleus.

Remember that the eigenstates of a single electron bound to a nucleus with charge $Z$ are the hydrogen levels ($\psi_n^Z = \psi_{1s}^Z, \psi_{2s}^Z, \psi_{2p}^Z, \dots$), except shrunken and shifted upward in binding energy ($E^Z$ more negative):

$$\mathcal{H}^Z \psi_n^Z = E_n^Z \psi_n$$
$$\psi_n^Z(\mathbf{r}) = \psi_n^H(\lambda_r \mathbf{r})$$
$$E^Z = \lambda_E E^H \tag{2}$$

(a) *By what factor $\lambda_r$ do the wavefunctions shrink? By what factor $\lambda_E$ do the energies grow?* (Hint: Dimensional arguments are preferred over looking up the formulas.)

In the independent electron approximation, the many-body electron eigenstates are created from products of single-electron eigenstates. The Pauli exclusion principle (which appears only useful in this independent electron approximation) says that exactly two electrons can fill each of the single-particle states.

(b) *Ignoring identical particle statistics, show that a product wavefunction*

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \dots) = \psi_{n_1}^Z(\mathbf{r}_1)\psi_{n_2}^Z(\mathbf{r}_2)\psi_{n_3}^Z(\mathbf{r}_3)\dots \tag{3}$$

*has energy $E = \sum_i E_{n_i}^Z$.*

The effect of the electron-electron repulsion in principle completely destroys this product structure. But for ground-state and excited-state quantum numbers, the language of filling independent electron orbitals is quite useful.[2] However, the energies of these states are strongly corrected by the interactions between the other electrons.

(c) *Consider the 2s and 2p states of an atom with a filled 1s shell (one electron of each spin in 1s states). Which state feels a stronger Coulomb attraction from the nucleus? Argue heuristically that the 2s state will generally have lower (more negative) energy and fill first.*

Let's check something I asserted, somewhat tentatively, in lecture. There I said that, for atoms with little spin-orbit coupling, the ground state wavefunction can be factored into a spatial and a spin piece:

$$\Psi(\mathbf{r}_1, s_1; \mathbf{r}_2, s_2; \mathbf{r}_3, s_3; \dots) \stackrel{?}{=} \psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3 \dots)\chi(s_1, s_2, s_3 \dots) \tag{4}$$

We'll check this in the first non-trivial case – the lithium atom ground state, in the independent electron approximation. From part (c), we know that two electrons should

---

[2]The excited states of an atom aren't energy eigenstates, they are *resonances*, with a finite lifetime. If you think of starting with the independent electron eigenstates and gradually turning on the Coulomb interaction and the interaction with photons, the true ground state and the resonances are adiabatic continuations of the single-particle product eigenstates – inheriting their quantum numbers.

occupy the 1s orbital, and one electron should occupy the 2s orbital. The two spins in the 1s orbital must be antiparallel; let us assume the third spin is pointing up $\uparrow_3$:

$$\Psi^0(\mathbf{r}_1, s_1; \mathbf{r}_2, s_2; \mathbf{r}_3, s_3) = \psi_{1s}^{\mathrm{Li}}(\mathbf{r}_1)\psi_{1s}^{\mathrm{Li}}(\mathbf{r}_2)\psi_{2s}^{\mathrm{Li}}(\mathbf{r}_3) \uparrow_1\downarrow_2\uparrow_3 . \tag{5}$$

But this combination is not antisymmetric under permutations of the electrons.

(d) *Antisymmetrize $\Psi^0$ with respect to electrons 1 and 2. Show that the resulting state is a singlet with respect to these two electrons. Antisymmetrize $\Psi^0$ with respect to all three electrons (a sum of six terms). Does it go to zero (in some obvious way)? Can it be written as a product as in eqn 4?*

5.8 **Three particles in a box.** (Quantum) ③

(Adapted from Sakurai, p. 4.1)

Consider free, noninteracting particles of mass $m$ in a one-dimensional box of length $L$ with infinitely high walls.

(a) *What are the lowest three energies of the single-particle energy eigenstates?*

If the particles are assumed non-interacting, the quantum eigenstates can be written as suitably symmetrized or antisymmetrized single-particle eigenstates. One can use a level diagram, such as in Fig. 1, to denote the fillings of the single particle states for each many-electron eigenstate.
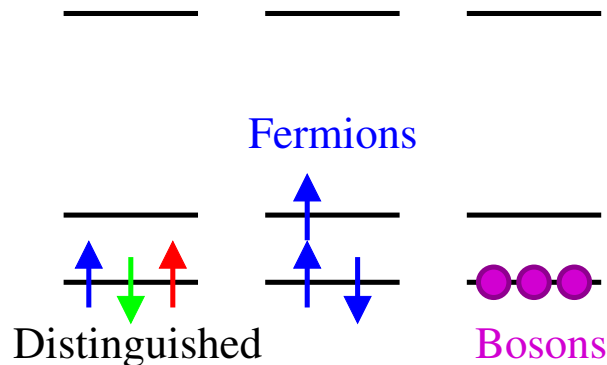


**Fig. 1 Level diagram**, showing one of the ground states for each of the three cases.

(b) *If three distinguishable spin-1/2 particles of the same mass are added to the box, what is the energy of the three-particle ground state? What is the degeneracy of the ground state? What is the first three-particle energy eigenvalue above the ground state? Its degeneracy? The degeneracy and energy of the second excited state? Draw a level diagram for one of the first excited states, and one of the second excited states (the ground state being shown on the left in Fig. 1).*

(c) *The same as part (b), but for three identical spin-1/2 fermions.*

(d) *The same as part (b), but for three identical spin-zero bosons.*

5.9 **Superfluids part II: ODLRO and broken gauge symmetry.** (Condensed matter, Quantum) ⑤

(Optional: Extra credit)

This second portion of the superfluid exercise introduces broken gauge symmetry, and deduces that a subvolume of a superfluid is best described as a superposition of states with different numbers of particles. You'll likely need to consult part I for context.

*Number conservation and $\psi$.* Figure 2 illustrates the fact that the local number of particles in a subvolume of a superfluid is indeterminate. Our ground state locally violates conservation of particle number.[3] If the number of particles in a local region is not well defined, perhaps we can think of the local state as some kind of superposition of states with different particle number? Then we could imagine factoring the off-diagonal long-range order $\langle a^\dagger(\mathbf{r}')a(\mathbf{r})\rangle \sim \psi^*(\mathbf{r}')\psi(\mathbf{r})$ into $\langle a^\dagger(\mathbf{r}')\rangle\langle a(\mathbf{r})\rangle$, with $\psi(\mathbf{r}) = \langle a\rangle$. (This is zero in a closed system, since $a(\mathbf{r})$ changes the total number of particles.) The immediate question is how to set the relative phases of the parts of the wavefunction with differing numbers of particles. Let us consider a region small enough that we can ignore the spatial variations.
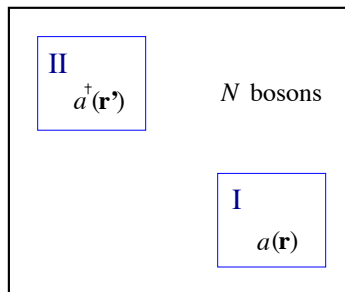


**Fig. 2 Delocalization and ODLRO**. Particles in superfluids are delocalized: the number of particles in a subvolume is not well defined. Annihilating a boson at $\mathbf{r}$ in region I, insofar as the boson comes out of the condensate, is equivalent to annihilating it at $\mathbf{r}'$. The probability overlap between these two states is precisely $\hat{\rho}_2(\mathbf{r}', r) = \psi^*(\mathbf{r}')\psi(\mathbf{r})$.

---

[3]This is not just the difference between canonical and grand canonical ensembles. Grand canonical ensembles are probability mixtures between states of different numbers of particles; superfluids have a coherent superposition of wavefunctions with different numbers of particles.

(d) *Consider a zero-temperature Bose condensate of $N$ non-interacting particles in a local region. Let the state into which the bosons condense, $\chi(\mathbf{r}) = \chi = |\chi| \exp(i\phi)$, be spatially uniform. What is the phase of the $N$-particle Bose-condensed state?*

The phase $\exp(i\phi(\mathbf{r}))$ is the relative phase between the components of the local Bose condensates with $N$ and $N-1$ particles. The superfluid state is a *coherent superposition of states with different numbers of particles* in local regions. How odd!

Momentum conservation comes from translational symmetry; energy conservation comes from time translational symmetry; angular momentum conservation comes from rotational symmetry. What symmetry leads to number conservation?

(e) *Consider the Hamiltonian $\mathcal{H}$ for a system that conserves the total number of particles, written in second quantized form (in terms of creation and annihilation operators). Argue that the Hamiltonian is invariant under a global symmetry which multiplies all of the creation operators by $\exp(i\zeta)$ and the annihilation operators by $\exp(-i\zeta)$. (This amounts to changing the phases of the $N$-particle parts of the wavefunction by $\exp(iN\zeta)$. Hint: Note that all terms in $\mathcal{H}$ have an equal number of creation and annihilation operators.)*

The magnitude $|\psi(\mathbf{r})|^2$ describes the superfluid density $n_s$. As we saw above, $n_s$ is the whole density for a zero-temperature non-interacting Bose gas; it is about one per cent of the density for superfluid helium, and about $10^{-8}$ for superconductors. If we write $\psi(\mathbf{r}) = \sqrt{n_s(\mathbf{r})} \exp(i\phi(\mathbf{r}))$, then the phase $\phi(\mathbf{r})$ labels which of the broken-symmetry ground states we reside in.[4]

*Broken gauge invariance.* We can draw a deep connection with quantum electromagnetism by promoting this global symmetry into a local symmetry. Consider the effects of shifting $\psi$ by a spatially-dependent phase $\zeta(x)$. It will not change the potential energy terms, but will change the kinetic energy terms because they involve gradients. Consider the case of a single-particle pure state. Our wavefunction $\chi(x)$ changes into $\widetilde{\chi} = \exp(i\zeta(x))\chi(x)$, and $[p^2/2m]\,\widetilde{\chi} = [((\hbar/i)\nabla)^2/2m]\,\widetilde{\chi}$ now includes terms involving $\nabla\zeta$.

(f) *Show that this single-particle Hamiltonian is invariant under a transformation which changes the phase of the wavefunction by $\exp(i\zeta(x))$ and simultaneously replaces $p$ with $p - \hbar\nabla\zeta$.*

This invariance under multiplication by a phase is closely related to gauge invariance in electromagnetism. Remember in classical electromagnetism the vector potential $\mathbf{A}$ is arbitrary up to adding a gradient of an arbitrary function $\Lambda$: changing $\mathbf{A} \to \mathbf{A} + \nabla\Lambda$ leaves the magnetic field unchanged, and hence does not change anything physical. There choosing a particular $\Lambda$ is called choosing a *gauge*, and this arbitrariness is

---

[4] $\psi(\mathbf{r})$ is the Landau order parameter; the phase $\phi(\mathbf{r})$ is the topological order parameter.

called *gauge invariance.* Also remember how we incorporate electromagnetism into the Hamiltonian for charged particles: we change the kinetic energy for each particle of charge $q$ to $(p - (q/c)A)^2/2m$, using the 'covariant derivative' $(\hbar/\mathrm{i})\nabla - (q/c)A$.

In quantum electrodynamics, particle number is not conserved, but charge is conserved. Our local symmetry, stemming from number conservation, is analogous to the symmetry of electrodynamics when we multiply the wavefunction by $\exp(\mathrm{i}(q/c)\zeta(x))$, where $q = -e$ is the charge on an electron.

(g) *Consider the Hamiltonian for a charged particle in a vector potential $H = ((\hbar/\mathrm{i})\nabla - (q/c)A)^2/2m + V(x)$. Show that this Hamiltonian is preserved under a transformation which multiplies the wavefunction by $\exp(\mathrm{i}(q/e)\zeta(x))$ and performs a suitable gauge transformation on A. What is the required gauge transformation?*

To summarize, we found that superconductivity leads to a state with a local indeterminacy in the number of particles. We saw that it is natural to describe local regions of superfluids as coherent superpositions of states with different numbers of particles. The order parameter $\psi(\mathbf{r}) = \langle a(\mathbf{r}) \rangle$ has amplitude given by the square root of the superfluid density, and a phase $\exp(\mathrm{i}\phi(\mathbf{r}))$ giving the relative quantum phase between states with different numbers of particles. We saw that the Hamiltonian is symmetric under uniform changes of $\phi$; the superfluid ground state breaks this symmetry just as a magnet might break rotational symmetry. Finally, we saw that promoting this global symmetry to a local one demanded changes in the Hamiltonian completely analogous to gauge transformations in electromagnetism; number conservation comes from a gauge symmetry. Superfluids spontaneously break gauge symmetry!

In Anderson's articles you can find more along these lines. In particular, number $N$ and phase $\phi$ turn out to be conjugate variables. The implied equation $\mathrm{i}\hbar\dot{N} = [\mathcal{H}, N] = \mathrm{i}\partial\mathcal{H}/\partial\phi$ gives the Josephson current, and is also related to the the equation for the superfluid velocity we derived in Exercise (2.5)