Problem Set 9: Groups & Representations
Graduate Quantum I
Physics 6572

James Sethna
Due Friday Oct. 24
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Potentially useful reading

Landau & Lifshitz *Quantum Mechanics*, ch. 12 (Group representations)
Sakurai and Napolitano, sections 7.1-7.2 (identical particles)
Schumacher & Westmoreland 14.3 (identical particles)
Weinberg section 4.5 (bosons & fermions)
Arfkin, Weber, and Harris, *Mathematical Methods for Physicists*, chapter 17 (Group representations)
Sethna [ignore temperature] sections 7.3 (bosons and fermions), 7.4 (non-interacting).

9.1 **Light Proton Superfluid.** (Dimensional Analysis) ③

In this exercise, we yet again examine a parallel world where the proton and neutron masses are equal to the electron mass, instead of ∼2000 times larger.

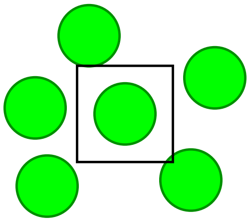

Fig. 1 Atoms with imaginary box of size equal to average space per atom

Atoms Bose condense when the number density n is high and the temperature T is low. One can view this condensation point as where temperature and the confinement energy become competitive. Up to a constant of order one, the thermal energy at the transition temperature $k_B T_c$ equals the confinement energy needed to put a helium atom in a box with impenetrable walls of length the mean nearest-neighbor spacing $L = n^{-1/3}$.

Calculate the ratio of the confinement energy $E_{\mathrm{He,ours}}$ *of Helium in our world and water* $E_{\mathrm{H_2O,light}}$ *in the parallel world.* Helium goes superfluid at $\sim 2^\circ K$ in our universe. *From that, estimate the superfluid transition temperature* T_c *for water in the parallel universe. Will it be superfluid at room temperature?* (Assume the box sizes for He in our world and water in the parallel world are the same.[1] Room temperature is about

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[1] The number of molecules of water per unit volume is comparable to the number of atoms of liquid helium per unit volume in the real world, and the water molecule will stay about the same size in the parallel world.

$300°K$. Helium 4, the isotope that goes superfluid, has two neutrons and two protons, with roughly equal masses. Oxygen 16 has eight protons, eight neutrons, and eight electrons.)

9.2 **Rotating Fermions.** (Group theory) ③

In this exercise, we'll explore the *geometry* of the space of rotations.

Spin 1/2 fermions transform upon rotations under $SU(2)$, the unitary 2×2 matrices with determinant one. Vectors transform under $SO(3)$, the ordinary 3×3 rotation matrices you know of.

Sakurai argues that a general $SU(2)$ matrix $U = \left(\begin{smallmatrix} a & b \\ -b^* & a^* \end{smallmatrix}\right)$ with $|a|^2 + |b|^2 = 1$. Viewing $\{\mathrm{Re}(a), \mathrm{Im}(a), \mathrm{Re}(b), \mathrm{Im}(b)\}$ as a vector in four dimensions, $SU(2)$ then geometrically is the unit sphere $\mathbb{S}^3$ in $\mathbb{R}^4$.

Remember that for every matrix R in $SO(3)$, there are two unitary matrices U and $-U$ corresponding to the same physical rotation. The matrix $-U$ has coordinates $(-a, -b)$ – it is the antipodal point on $\mathbb{S}^3$, exactly on the opposite side of the sphere. So $SO(3)$ is geometrically the unit sphere with *antipodal points identified.* This is called (for obscure reasons) the *projective plane*, $\mathbb{R}P^3$.

Feynman's plate (in Feynman's plate trick) as it rotates 360° travels in rotation space from one orientation to its antipode. While I'm not sure anyone has figured out whether arms, shoulders, and elbows duplicate the properties of fermions under rotations, the plate motion illustrates the possibility of a minus sign.

But we can calculate this trajectory rather neatly by mapping the rotations not to the unit sphere, but to the space $\mathbb{R}^3$ of three-dimensional vectors. (Just as the 2-sphere $\mathbb{S}^2$ can be projected onto the plane, with the north pole going to infinity, so can the 3-sphere $\mathbb{S}^3$ be projected onto $\mathbb{R}^3$.) Remember the axis-angle variables, where a rotation of angle ϕ about an axis $\hat{\mathbf{n}}$ is given by

$$\exp(-\mathrm{i}\mathbf{S} \cdot \hat{\mathbf{n}}\phi/\hbar) = \exp(-\mathrm{i}\boldsymbol{\sigma} \cdot \hat{\mathbf{n}}\phi/2) = \exp(-\mathrm{i}\mathbf{J} \cdot \hat{\mathbf{n}}\phi/\hbar) \tag{1}$$

where the middle formula works for $SU(2)$ (where $\mathbf{S} = \hbar\sigma/2$, because the particles have spin 1/2) and the last formula is appropriate for $SO(3)$.[2] We figure $\mathbf{n}$ will be the direction of the vector in $\mathbb{R}^3$ corresponding to the rotation, but how will the length depend on ϕ? Since all rotations by 360° are the same, it makes sense to make the length of the vector go to infinity as $\phi \to 360°$. We thus define the *Modified Rodrigues coordinates* for a rotation to be the vector $\mathbf{p} = \hat{\mathbf{n}} \tan(\phi/4)$.

(a) *Fermions, when rotated by 360°, develop a phase change of* $\exp(\mathrm{i}\pi) = -1$ *(as discussed in Sakurai & Napolitano p. 165, and as we illustrated with Feynman's plate*

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[2] The factor of two is there for $SU(2)$ because the spin is 1/2. For $SO(3)$, infinitesimal generators are antisymmetric matrices, so $\mathbf{S}^{(i)}_{jk} = \mathbf{J}^{(i)}_{jk} = \mathrm{i}\hbar\epsilon_{ijk}$ in the xyz basis; in the usual quantum basis $m_z = (-1, 0, 1)$ the formula will be different.

trick). Give the trajectory of the modified Rodrigues coordinate for the fermion's rotation as the plate is rotated $720°$ *about the axis* $\hat{\mathbf{n}} = \hat{z}$. (We want the continuous trajectory on the sphere $\mathbb{S}^3$, perhaps which passes through the point at ∞. Hint: The trajectory is already defined by the modified Rodrigues coordinate: just describe it.)

(b) *For a general Rodrigues point* $\mathbf{p}$ *parameterizing a rotation in* $SO(3)$*, what antipodal point* $\mathbf{p}'$ *corresponds to the same rotation?* (Hint: A rotation by ϕ and a rotation by $\phi + 2\pi$ should be identified.)

9.3 **Matrices, wavefunctions, and group representations.** (Group reps) ③

In this exercise, we shall explore the *tensor product* of two vector spaces, and how they transform under rotations. We'll draw analogies between two examples: vectors → matrices and single-particle-states → two-particle-wavefunctions.

The tensor product between two vectors is $(\mathbf{v} \otimes \mathbf{w})_{ij} = v_i w_j$. The tensor product between two single-particle wavefunctions $\zeta(x)$ for particle A and $\phi(y)$ for particle B is the product wavefunction $\Psi(x, y) = \zeta(x)\phi(y)$. If $H^{(A)}$ and $H^{(B)}$ are the Hilbert spaces for particles A and B, the tensor product space $H^{(AB)} = H^{(A)} \otimes H^{(B)}$ is the space of all linear combinations of tensor products $\Psi(x, y) = \zeta(x)\phi(y)$ of states in $H^{(A)}$ and $H^{(B)}$. Two-particle wavefunctions live in $H^{(AB)}$.

Let $\{\hat{\mathbf{e}}_i\} = \{\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3\}$ be an orthonormal basis for $\mathbb{R}^3$, and let $\{\zeta_\alpha\}$ and $\{\phi_\beta\}$ be orthonormal bases for the Hilbert spaces $H^{(A)}$ and $H^{(B)}$ for particles A and B.

(a) *Show that the tensor products* $\Psi_{\alpha\beta}(x, y) = \zeta_\alpha(x)\phi_\beta(y)$ *are orthonormal.* (The dot product is the usual $\int \mathrm{d}x\mathrm{d}y \Psi^*\Psi$.) With some more work, it is possible to show that they are also complete, forming an orthonormal basis of $H^{(AB)}$.)

Suppose the two particles are both in states with total angular momentum $L_A = L_B = 1$, and are then coupled with a small interaction. Angular momentum addition rules then say that the two-particle state can have angular momentum $L_{(AB)}$ equal to 2 or 1 or 0: $1 \otimes 1 = 2 \oplus 1 \oplus 0$. In group representation theory, this decomposition corresponds to finding three subspaces that are invariant under rotations.

The tensor product space $\mathbb{R}^3 \otimes \mathbb{R}^3$ are normally written as 3×3 matrices M_{ij}, where $M = \sum_{i=1}^{3}\sum_{j=1}^{3} M_{ij}\hat{\mathbf{e}}_i\hat{\mathbf{e}}_j$. Vectors transform under $L = 1$, so we would expect matrices to decompose into $L = 2$, 1, and 0.

(b) *Show that the antisymmetric matrices, the multiples of the identity matrix, and the traceless symmetric matrices are all invariant under rotation (i.e.,* $R^{-1}MR$ *is in the same subspace as* M *for any rotation* R*). Which subspace corresponds to which angular momentum?*

(c) *Consider the* $L = 1$ *subspace of matrices* M*. Using the totally antisymmetric tensor* ϵ_{ijk}*, map this subspace into vectors*[3] *in* $\mathbb{R}^3$*. Are these vectors or pseudovectors?*

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[3] It's important that the mapping behaves properly as the coordinates rotate. Because the tensor ϵ_{ijk} is rotation invariant (like δ_{ij}), any contraction of vectors or tensors with it will transform properly under rotations. That's why dot products $\mathbf{v} \cdot \mathbf{w} = \sum \delta ijv_i w_j$ and cross products $(\mathbf{v} \times \mathbf{w})_i = \sum \epsilon ijkv_j w_k$ are so common in physics – they transform correctly under rotations.

I always found torque $\boldsymbol{\tau} = \mathbf{r}\times\mathbf{F}$ quite mysterious. (Its direction depends on whether you are right- or left-handed!) If you calculate the torque as the antisymmetric 3×3 matrix $M_{ij} = r_i F_j - r_j F_i$ then this mystery disappears. It is convenient to turn antisymmetric 3×3 matrices into pseudovectors (especially for those who haven't had much math yet), but it can be physically somewhat confusing.

Thus the angular momentum addition rules for particles with angular momentum equal to one correspond nicely to the ways in which matrices and tensors can be decomposed into rotation-invariant subspaces.

Now suppose our two $L = 1$ particles are identical, with spins aligned.

(d) *Which total orbital angular momentum states are allowed for spin-aligned fermions? For spinless bosons?*

Many physical properties are described by symmetric matrices: the dielectric constant in electromagnetism, the stress and strain tensors in elastic theory, and so on.

9.4 **Crystal field theory: *d*-orbitals.** (Group reps) ③

The vector space of functions $f(x, y, z)$ on the unit sphere transforms into itself under rotations $f(\mathbf{x}) \to_R f(R^{-1}\mathbf{x})$. These transformations are linear $(af(\mathbf{x}) + g(\mathbf{x}) \to_R af(R^{-1}\mathbf{x}) + g(R^{-1}\mathbf{x}))$, and obey the group composition rule, and thus form a representation of the rotation group.

(a) *Argue that the homogeneous polynomials of degree ℓ,*

$$f(x, y, z) = \sum_{m=0}^{\ell} \sum_{n=0}^{\ell-m} f_{\ell mn} x^m y^n z^{\ell-m-n} \tag{2}$$

form a subspace that is invariant under rotations. (Hint: The three components of a rotation of $\{x, y, z\}$ are linear combinations of x, y, and z. Use the distributive property.)

Thus the irreducible representations are contained in these invariant subspaces. Sakurai indeed mentions in his section 3.11 on tensor operators that $Y_1^0 = \sqrt{3/4\pi}z/r$ and $Y_1^{\pm1} = \mp\sqrt{3/2\pi}(x \pm iy)/r$, and also gives a formula for $Y_2^{\pm2}$; since $r = 1$ on our unit sphere these are homogeneous polynomials of degree one.

(b) *Look up the $\ell = 2$ spherical harmonics (e.g. in Sakurai's appendix B) and write them as quadratic polynomials in x, y, and z.*

The $\ell = 2$ spherical harmonics are the angular parts of the wavefunctions for electrons in d orbitals (e.g. of transition metal atoms).[4] Electrons in d-orbitals are much more

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[4] Here we use the common independent-electron language, where the complex many-body wavefunction of an atom, molecule, or solid is viewed as filling single-electron states, even though the electron-electron repulsion is almost as strong as the electron-nuclear attraction. This idea can be dignified in three rather different ways. First, one can view each electron as feeling an effective potential given by the nucleus plus the average density of electrons. This leads to mean-field Hartree-Fock theory. Second, one can show that the

tightly contained near the nucleus than p and s orbitals of similar energy.[5] In molecules and solids, the s and p orbitals usually hybridize (superimpose) into chemical bonds and broad electron bands, where the original orbitals are strongly distorted. In contrast, d-electrons rarely participate in chemical bonds, and their electron bands are narrow – almost undistorted orbitals with small hopping rates. The energy levels of the five d-orbitals are, however, shifted from one another by their environments. (For crystals, these shifts are called *crystal field splittings.*)

We can use group representation theory to understand how the d-orbitals are affected by their molecular or crystalline environment.

First, we need to calculate the character $\chi(R) = \chi(\hat{n}, \phi)$ of the $\ell = 2$ representation. Remember that the character is the trace of the (here 5×5) matrix corresponding to the rotation. Remember that this trace depends only on the *conjugacy class* of R – that is, if S is some other group element then $\chi(S^{-1}RS) = \chi(R)$. Remember that any two rotations by the same angle ϕ are conjugate to one another.[6]

In class, we found that the character of the $\ell = 1$ representation by using the Cartesian x, y, z basis, where $R_{\hat{z}}(\phi) = \begin{pmatrix} \cos(\phi) & -\sin(\phi) & 0 \\ \sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & 1 \end{pmatrix}$. Hence $\chi^{(1)}(\phi) = 1 + 2\cos(\phi)$. We can do this same calculation in the m_z basis of the spherical harmonics, where Y_1^0 is unchanged under rotations and $Y_1^{\pm 1} \to \exp(\pm \mathrm{i}\phi) Y_1^{\pm 1}$. Here

$$\mathcal{D}^{(1)}_{\hat{z}}(\phi) = \begin{pmatrix} \exp(\mathrm{i}\phi) & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \exp(-\mathrm{i}\phi) \end{pmatrix}, \tag{3}$$

and again $\chi^{(1)}(\phi) = 1 + 2\cos(\phi)$.

(c) *Calculate $\mathcal{D}^{(2)}_{\hat{z}}(\phi)$, the transformation matrix for the $L = 2$ spherical harmonics under a rotation by ϕ about the z axis, in analogy with eqn 3. Calculate the character $\chi^{(2)}(\phi)$ of the $L = 2$ representation. Give the characters for rotations C_n by $2\pi/n$, for $n = 1$, 2, 3, and 4 (the important rotations for crystalline symmetry groups.)* (Hints: C_n is an n-fold axis of rotation, a rotation by $2\pi/n$.)

The most common symmetry groups for d-electron atoms in crystals is O, the octahedral group (the symmetry group of a cube). Here let us run through a tangible calculation, to learn how to use character tables to decompose representations. Look

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ground state energy can be written as an unknown functional of the electron density (the *Hohenberg-Kohn theorem*, and then calculate the kinetic energy terms as an effective single-body Schrödinger equation in the resulting effective potential due to the net electron density (the *Kohn-Sham equations*). Third, one can start with independent electrons (or Hartree-Fock electrons) and slowly 'turn on' the electron-electron repulsion. The independent-electron excited eigenstates develop lifetimes and become *resonances.* For atoms these lifetimes represent Auger decay rates. For crystals these resonances are called *quasiparticles* and the theory is called *Landau Fermi liquid theory.* Landau Fermi-liquid theory is usually derived using Greens functions and Feynman diagrams, but it has recently been re-cast as a renormalization-group flow.

[5] The d-orbitals have angular nodes in the wavefunction; the s and p orbitals of similar energy will have radial nodes in their wavefunctions that push the probability farther from the nucleus.

[6] If the two rotations have axes $\hat{n}$ and $\hat{n}'$, choose S to rotate $\hat{n}'$ into $\hat{n}$.

up the character tables for the irreducible representations of the finite group O. (To simplify the calculation, we'll assume that inversion symmetry is broken; otherwise we should use O_h, which has twice the number of group elements.)

(d) *Find a character table for the octahedral group* O. *It should have labels for the columns* E, $8C_3$, $3C_2$, $6C_2$, *and* $6C_4$. *The multipliers tell you how many group elements are in each conjugacy class. Describe in words what symmetry of the cube corresponds to each column. Why are there two different columns for two-fold rotations?* (Hint: Two rotations that are conjugate in $SO(3)$ need not be conjugate when restricted to O. Usually symmetries that are 'physically different' are in different conjugacy classes.)

As an example, we might imagine that p-electron orbitals will stay degenerate under a cubic perturbation.

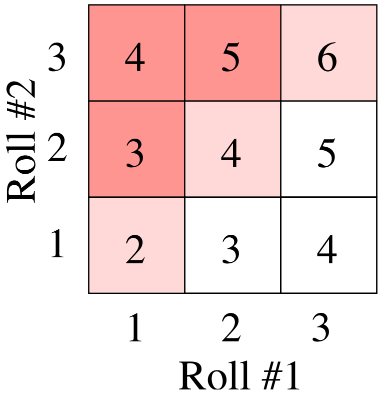
(e) *Verify that the characters,* $1 + 2\cos(\phi)$ *for the* $L = 1$ *representation in these five columns* $E \to 3$, $8C_3 \to 0$, $3C_2 \to -1$, $6C_2 \to -1$, *and* $6C_4 \to 1$ *are identical to one of the rows. Which three-dimensional irreducible representation of* O *is it?* (This means that the p-electron orbitals do indeed stay an irreducible representation when the spherical symmetry is broken down to cubic, and hence will stay degenerate.) *Check that our character is indeed orthogonal to the other rows in the table. Check that the 'dot product' of our character with the identical row is indeed the number of elements in the octahedral group,* $o(O) = 24$.

(f) *Use the orthogonality relations of the characters of irreducible representations for* O, *decompose the* $\ell = 2$ *representation from part (c) into irreducible representations of the octahedral group. How will the energies of the single-particle d-orbitals of a transition metal atom split in an octahedral environment? What will the degeneracies and symmetries* (A_1, A_2, E, …) *be of the different levels?* (Hints: (1) C_n is an n-fold axis of rotation, a rotation by $2\pi/n$. (2) When you take the dot product of your character from part (c) with the row, make sure you multiply by the number of elements in the conjugacy class. If you are doing it right, the dot product of the characters should equal a multiple of the number of octahedral group elements $o(O) = 24$, and the dimensions of the sub-representations should add up to five.)

This may seem like magic. Let's pull it down to earth, by identifying which d orbitals are in which of the irreducible representations. Your answer to part (d) should have involved one two-dimensional irreducible representation and one three-dimensional one. The five d-orbitals are often denoted d_{xy}, d_{xz}, d_{yz}, d_{z^2} and $d_{x^2-y^2}$. (This is a bit of a cheat; really d_{z^2} should be written $d_{2z^2-x^2-y^2}$ or something like that.) This particular basis is nice, because the cubic rotations acting in this basis are block-diagonal. Translated into group representation lingo, this means three of these elements form an invariant subspace, and the other two form another invariant subspace.

(g) *Figure out which of these orbitals are in each of the two representations you found in part (d).* (Hint: Check how these five orbitals transform under the octahedral symmetries that permute x, y, and z among themselves.)

9.5 **Quantum dice.**[7] (Quantum) ②



Roll #2			
3	4	5	6
2	3	4	5
1	2	3	4
	1	2	3
	Roll #1		

Fig. 2 Quantum dice. Rolling two dice. In *Bosons*, one accepts only the rolls in the shaded squares, with equal probability 1/6. In *Fermions*, one accepts only the rolls in the darkly-shaded squares (not including the diagonal from lower left to upper right), with probability 1/3.

You are given several unusual 'three-sided' dice which, when rolled, show either one, two, or three spots. There are three games played with these dice: *Distinguishable*, *Bosons*, and *Fermions*. In each turn in these games, the player rolls one die at a time, starting over if required by the rules, until a legal combination occurs. In *Distinguishable*, all rolls are legal. In *Bosons*, a roll is legal only if the new number is larger or equal to the preceding number. In *Fermions*, a roll is legal only if the new number is strictly larger than the preceding number. See Fig. 2 for a table of possibilities after rolling two dice.

Our dice rules are the same ones that govern the quantum statistics of identical particles.

(a) *Presume the dice are fair: each of the three numbers of dots shows up* $1/3$ *of the time. For a legal turn rolling a die twice in Bosons, what is the probability* $\rho(4)$ *of rolling a 4? Similarly, among the legal Fermion turns rolling two dice, what is the probability* $\rho(4)$*?*

(b) *For a legal turn rolling three 'three-sided' dice in Fermions, what is the probability* $\rho(6)$ *of rolling a 6?* (Hint: There is a Fermi exclusion principle: when playing *Fermions*, no two dice can have the same number of dots showing.) Electrons are fermions; no two electrons can be in exactly the same state.

When rolling two dice in *Bosons*, there are six different legal turns (11), (12), (13), . . . , (33); half of them are doubles (both numbers equal), while for plain old *Distinguishable* turns only one-third would be doubles[8]; the probability of getting doubles is enhanced

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[7] This exercise was developed in collaboration with Sarah Shandera.

[8] For *Fermions*, of course, there are no doubles.

by 1.5 times in two-roll *Bosons*. When rolling three dice in *Bosons*, there are ten different legal turns (111), (112), (113), ..., (333). When rolling M dice each with N sides in *Bosons*, one can show that there are

$$\binom{N+M-1}{M} = \frac{(N+M-1)!}{M!\,(N-1)!}$$

legal turns.

(c) *In a turn of three rolls, what is the factor by which the probability of getting triples in Bosons is enhanced over that in Distinguishable? In a turn of M rolls, what is the enhancement factor for generating an M-tuple (all rolls having the same number of dots showing)?*

Notice that the states of the dice tend to cluster together in *Bosons*. Examples of real bosons clustering into the same state include Bose condensation and lasers (future exercies).

9.6 **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. 3, to denote the fillings of the single particle states for each many-electron eigenstate.

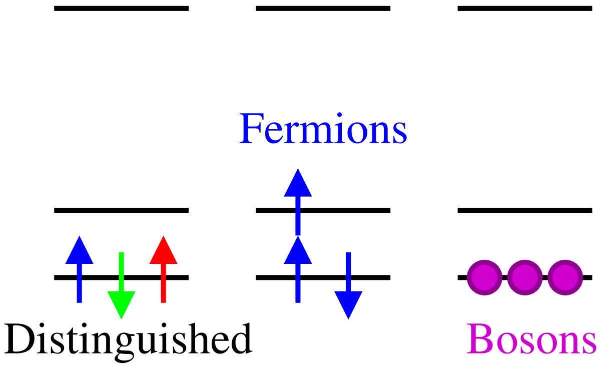

Fig. 3 Level diagram, showing one of the ground states for each of the three cases.

(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. 3).*

(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.*