Problem Set 6: Group representation theory and neutron stars
Graduate Quantum I
Physics 6572

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Reading

Sakurai and Napolitano, section 3.11, 5.9, and 7.5
Landau & Lifschitz *Quantum Mechanics*, chapter 12 sections 91-96.

Further reading

Morton Hamermesh, *Group theory and its application to physical problems*

6.1 **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 $\{\hat{\mathbf{e}}_i\} = \{\hat{x}, \hat{y}, \hat{z}\}$ be an orthonormal basis for $\mathbb{R}^3$, and let $\{\zeta_i\}$ and $\{\phi_j\}$ be orthonormal bases for the Hilbert spaces $H^{(A)}$ and $H^{(B)}$ for particles A and B.

(a) *Show that the tensor products $\Psi_{ij}(x, y) = \zeta_i(x)\phi_j(y)$ 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. Provide the (standard) formula taking this space into vectors in $\mathbb{R}^3$. Why are these called pseudovectors?*

I always found torque $\boldsymbol{\tau} = \mathbf{r} \times \mathbf{F}$ quite mysterious. (Its direction depends on whether you are right- or left-handed!) Fundamentally, we see now that this is because torque isn't a vector – it is an antisymmetric 3×3 matrix.

How does this relate back to quantum wavefunctions? Suppose our two $L = 1$ particles are identical, with spins in the same state.

(d) *Which angular momentum states are allowed for spin-aligned fermions? For spin-aligned or 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.

6.2 **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 $f(\mathbf{x}) \rightarrow_R f(R^{-1}\mathbf{x})$. These transformations are linear ($af(\mathbf{x}) + g(\mathbf{x}) \rightarrow_R af(R^{-1}\mathbf{x}) + g(R^{-1}\mathbf{x})$), and obey the group composition rule, and thus form a representation of the rotation group.

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

$$f(x, y, z) = \sum_{m=0}^{\ell} \sum_{n=0}^{\ell-m} f_{\ell mn} x^m y^n z^{\ell-m-n} \tag{1}$$

form a subspace that is invariant under rotations.

Thus the irreducible representations are contained in these invariant subspaces. Sakurai indeed mentions in his section 3.11 on tensor operators that $Y_1^0 = \sqrt{3/\pi}z/r$ and $Y_1^{\pm 1} = \sqrt{3/2\pi}(x \pm iy)/r$, and also gives a formula for $Y_2^{\pm 2}$; 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).[1] Electrons in d-orbitals are much more

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[1] 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 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

tightly contained near the nucleus than p and s orbitals. 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.[2]

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 $R_{\hat{z}}(\phi) = \begin{pmatrix} \exp(\mathrm{i}\phi) & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \exp(-\mathrm{i}\phi) \end{pmatrix}$, and again $\chi^{(1)}(\phi) = 1 + 2\cos(\phi)$.

(c) *Calculate* $\chi^{(2)}(\phi)$. *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.)*

The most common symmetry groups for d-electron atoms in crystals is O, the octahedral group (the symmetry group of a cube). Look up the character tables for the irreducible representations of this finite group. (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) *Use the orthogonality relations of the characters of irreducible representations for* O, *decompose the* $\ell = 2$ *representation above 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?* (Hint: If you are doing it right, the dot product of the characters should equal a multiple of the number of octahedral

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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.

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

group elements $o(O) = 24$, and the dimensions of the sub-representations should add up to five.)

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.

(e) *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.)

6.3 **White dwarfs, neutron stars, and black holes.** (Astrophysics, Quantum) ③

As the energy sources in large stars are consumed, and the temperature approaches zero, the final state is determined by the competition between gravity and the chemical or nuclear energy needed to compress the material.

A simplified model of ordinary stellar matter is a Fermi sea of non-interacting electrons, with enough nuclei to balance the charge. Let us model a white dwarf (or black dwarf, since we assume zero temperature) as a uniform density of He^4 nuclei and a compensating uniform density of electrons. Assume Newtonian gravity. Assume the chemical energy is given solely by the energy of a gas of non-interacting electrons (filling the levels to the Fermi energy).

(a) *Assuming non-relativistic electrons, calculate the energy of a sphere with N zero-temperature non-interacting electrons and radius R.*[3] *Calculate the Newtonian gravitational energy of a sphere of* He^4 *nuclei of equal and opposite charge density. At what radius is the total energy minimized?*

A more detailed version of this model was studied by Chandrasekhar and others as a model for white dwarf stars. Useful numbers: $m_p = 1.6726 \times 10^{-24}\,\mathrm{g}$, $m_n = 1.6749 \times 10^{-24}\,\mathrm{g}$, $m_e = 9.1095 \times 10^{-28}\,\mathrm{g}$, $\hbar = 1.05459 \times 10^{-27}\,\mathrm{erg\,s}$, $G = 6.672 \times 10^{-8}\,\mathrm{cm}^3/(\mathrm{g\,s}^2)$, $1\,\mathrm{eV} = 1.60219 \times 10^{-12}\,\mathrm{erg}$, $k_B = 1.3807 \times 10^{-16}\,\mathrm{erg/K}$, and $c = 3 \times 10^{10}\,\mathrm{cm/s}$.

(b) *Using the non-relativistic model in part (a), calculate the Fermi energy of the electrons in a white dwarf star of the mass of the Sun,* 2×10^{33} *g, assuming that it is composed of helium.* (i) *Compare it to a typical chemical binding energy of an atom. Are we justified in ignoring the electron–electron and electron–nuclear interactions (i.e., chemistry)?* (ii) *Compare it to the temperature inside the star, say* $10^7\,\mathrm{K}$*. Are we justified in assuming that the electron gas is degenerate (roughly zero temperature)?* (iii) *Compare it to the mass of the electron. Are we roughly justified in using a non-relativistic theory?* (iv) *Compare it to the mass difference between a proton and a neutron.*

The electrons in large white dwarf stars are relativistic. This leads to an energy which grows more slowly with radius, and eventually to an upper bound on their mass.

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[3] You may assume that the single-particle eigenstates have the same energies and **k**-space density in a sphere of volume V as they do for a cube of volume V; just like fixed versus periodic boundary conditions, the boundary does not matter to bulk properties.

(c) *Assuming extremely relativistic electrons with* $\varepsilon = pc$*, calculate the energy of a sphere of non-interacting electrons. Notice that this energy cannot balance against the gravitational energy of the nuclei except for a special value of the mass,* M_0*. Calculate* M_0*. How does your* M_0 *compare with the mass of the Sun, above?*

A star with mass larger than M_0 continues to shrink as it cools. The electrons (see (iv) in part (b) above) combine with the protons, staying at a constant density as the star shrinks into a ball of almost pure neutrons (a *neutron star*, often forming a *pulsar* because of trapped magnetic flux). Recent speculations suggest that the 'neutronium' will further transform into a kind of quark soup with many strange quarks, forming a transparent insulating material.

For an even higher mass, the Fermi repulsion between quarks cannot survive the gravitational pressure (the quarks become relativistic), and the star collapses into a black hole. At these masses, general relativity is important, going beyond the purview of this text. But the basic competition, between degeneracy pressure and gravity, is the same.