University of California at San Diego – Department of Physics – Prof. John McGreevy

Physics 212C QM Spring 2023
Assignment 6 – Solutions

Due 11:00am Wednesday, May 17, 2023

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1. **Brain-warmer.** Consider two single-particle orbitals with wavefunctions $\psi_\alpha(r), \psi_\beta(r)$. Find the position-space wavefunctions

$$\Psi(r_1\sigma, r_2\sigma') \equiv \langle r_1\sigma, r_2\sigma'|\Psi\rangle = \langle 0| \mathbf{a}_{r_2\sigma'}\mathbf{a}_{r_1\sigma} |\Psi\rangle$$

for the four states of two spinful fermions:

$$|S\rangle = \frac{1}{\sqrt{2}}\mathbf{a}^\dagger_{\alpha\sigma}\mathbf{a}^\dagger_{\beta\sigma'}\varepsilon_{\sigma\sigma'}|0\rangle = \frac{1}{\sqrt{2}}\left(\mathbf{a}^\dagger_{\alpha\uparrow}\mathbf{a}^\dagger_{\beta\downarrow} - \mathbf{a}^\dagger_{\alpha\downarrow}\mathbf{a}^\dagger_{\beta\uparrow}\right)|0\rangle$$

$$|A,1\rangle = \mathbf{a}^\dagger_{\alpha\uparrow}\mathbf{a}^\dagger_{\beta\uparrow}|0\rangle, \quad |A,0\rangle = \frac{1}{\sqrt{2}}\left(\mathbf{a}^\dagger_{\alpha\uparrow}\mathbf{a}^\dagger_{\beta\downarrow} + \mathbf{a}^\dagger_{\alpha\downarrow}\mathbf{a}^\dagger_{\beta\uparrow}\right)|0\rangle, \quad |A,-1\rangle = \mathbf{a}^\dagger_{\alpha\downarrow}\mathbf{a}^\dagger_{\beta\downarrow}|0\rangle.$$

Check that the singlet (triplet) indeed has a symmetric (antisymmetric) orbital wavefunction. Check that the labels on the A states correctly label the eigenvalues of the total spin along z, $S^z \equiv \sum_r \frac{1}{2}\mathbf{a}^\dagger_r\sigma^z\mathbf{a}_r$.

To find the wavefunctions, we can use equation 1.23 from the lecture notes: $\mathbf{a}^\dagger_{\alpha\sigma} = \sum_r \mathbf{a}^\dagger_{r\sigma}\psi_\alpha(r)$. This gives

$$\langle r_1\sigma, r_2\sigma'|S\rangle \equiv \frac{1}{\sqrt{2}}\langle 0|\mathbf{a}_{r_1\sigma}\mathbf{a}_{r_2\sigma'}|S\rangle = \Psi_S(r_1,r_2)\left(\delta_{\sigma\uparrow}\delta_{\sigma'\downarrow} - \delta_{\sigma\downarrow}\delta_{\sigma'\uparrow}\right)/\sqrt{2}.$$

$$\langle r_1\sigma, r_2\sigma'|A,0\rangle \equiv \frac{1}{\sqrt{2}}\langle 0|\mathbf{a}_{r_1\sigma}\mathbf{a}_{r_2\sigma'}|A,0\rangle = \Psi_A(r_1,r_2)\left(\delta_{\sigma\uparrow}\delta_{\sigma'\downarrow} + \delta_{\sigma\downarrow}\delta_{\sigma'\uparrow}\right)/\sqrt{2}.$$

$$\langle r_1\sigma, r_2\sigma'|A,1\rangle \equiv \frac{1}{\sqrt{2}}\langle 0|\mathbf{a}_{r_1\sigma}\mathbf{a}_{r_2\sigma'}|A,1\rangle = \Psi_A(r_1,r_2)(\delta_{\sigma\uparrow}\delta_{\sigma'\uparrow}).$$

$$\langle r_1\sigma, r_2\sigma'|A,-1\rangle \equiv \frac{1}{\sqrt{2}}\langle 0|\mathbf{a}_{r_1\sigma}\mathbf{a}_{r_2\sigma'}|A,1\rangle = \Psi_A(r_1,r_2)(\delta_{\sigma\downarrow}\delta_{\sigma'\downarrow}).$$

So indeed the triplet has a symmetric orbital wavefunction, and the states have $S^z = 0, \pm 1$ respectively.

2. **Brain-warmer: a beam of particles.** Suppose the occupation numbers for a state of bosons satisfy

$$n_{\vec{p}} = ce^{-\alpha(\vec{p}-\vec{p}_0)^2/2}.$$

(a) Determine the prefactor $c = c(n, \alpha, p_0)$ so that the average density is

$$n = \int đ^3 p n_{\vec{p}}.$$

$$n = c \int đ^3 p e^{-\alpha(p-p_0)^2/2} = \sqrt{\frac{\pi}{2}} \frac{c}{\alpha^{3/2}} \frac{4\pi}{(2\pi)^3}$$
$$\implies c = n(2\pi\alpha)^{3/2}.$$

(b) Check that with this normalization, in the thermodynamic limit of $N \to \infty$ at fixed $n = N/V$, the pair correlation function is

$$g(x-y) = 1 + e^{-(x-y)^2/\alpha}.$$

In this limit we can ignore the correction to Wick's theorem. By translation invariance, the pair correlation function only depends on the separation, which we'll call x:

$$g_B(x) = \frac{1}{n^2}\left(n^2 + |\int đ^3 p n_p e^{-\mathbf{i}p\cdot x}|^2\right) = 1 + |X|^2$$

with

$$X = \int đ^3 p c e^{-\frac{\alpha}{2}\left(p^2 - 2p\cdot q\right) - \frac{\alpha p_0^2}{2}}, \quad q \equiv p_0 - \mathbf{i}x/\alpha \tag{1}$$

$$= \underbrace{c \int đ^3 k e^{-\frac{\alpha}{2}k^2}}_{=n} e^{-\frac{\alpha}{2}\left(p_0^2 - q^2\right)} \tag{2}$$

$$= n e^{-\mathbf{i}p_0 x - \frac{x^2}{2\alpha}} \quad . \tag{3}$$

Therefore

$$g_B(x) = 1 + e^{-\frac{x^2}{\alpha}}$$

as promised.

3. **Density matrix and correlation functions.** Consider the single-particle density matrix in a mixed state $\rho = \sum_s p_s |\Psi_s\rangle\langle\Psi_s|$ of N particles, defined as

$$\rho_1(r, r') \equiv \sum_s p_s \sum_{r_2..r_N} \Psi_s^\star(r, r_2, \cdots r_N)\Psi_s(r', r_2, \cdots r_N).$$

This can be defined for either bosons or fermions.

(a) Check that ρ_1 is proportional to the two-point correlation function

$$\rho_1(r,r') \propto \mathrm{tr}\rho\psi^\dagger(r)\psi(r') \equiv \left\langle \psi^\dagger(r)\psi(r')\right\rangle$$

and find the proportionality constant. Check that it works for both bosons and fermions.

Using $|\Psi\rangle = \sum_{r_1\cdots r_N} \Psi(r_1\cdots r_N)\,|r_1\cdots r_N\rangle$ and

$$\psi(r)\,|r_1\cdots r_N\rangle = \frac{1}{\sqrt{n}}\left(\delta(r-r_n)\,|r_1\cdots r_{n-1}\rangle + \zeta\delta(r-r_{n-1})\,|r_1\cdots r_{n-2}r_n\rangle \right. \\ \left. + \cdots \zeta^{n-1}\delta(r-r_1)\,|r_2\cdots r_n\rangle\right) \tag{4}$$

we have

$$\langle\Psi|\,\psi^\dagger(r)\psi(r')\,|\Psi\rangle \tag{5}$$
$$= \sum_{r_1\cdots r_N}\sum_{r_1'\cdots r_N'} \Psi^\star(r_1\cdots r_N)\Psi(r_1'\cdots r_N')\,\langle r_1\cdots r_N|\,\psi^\dagger(r)\psi(r')\,|r_1'\cdots r_N'\rangle \tag{6}$$

$$\langle r_1\cdots r_N|\,\psi^\dagger(r)\psi(r')\,|r_1'\cdots r_N'\rangle \tag{7}$$
$$= \frac{1}{N}\sum_{i=1}^{N}\zeta^i\sum_{j=1}^{N}\zeta^j\delta^d(r-r_i)\delta^d(r'-r_j')\left\langle r_1\cdots\widehat{r_i}\cdots r_N|r_1'\cdots\widehat{r_j'}\cdots r_N'\right\rangle \tag{8}$$
$$= \frac{1}{N}\sum_{i=1}^{N}\zeta^i\sum_{j=1}^{N}\zeta^j\delta^d(r-r_i)\delta^d(r'-r_j')\cdot \tag{9}$$
$$\frac{1}{(N-1)!}\sum_{\pi\in S_{N-1}}\zeta^\pi\delta^d(r_1-r'_{\pi(1)})\cdots\delta(\widehat{r_i-r_{\pi(i)'}})\delta^d(r_N-r'_{\pi(N)})$$

(note that there is no delta function involving r_j', so there are $N-1$ delta functions). Now, plugging this into the sum over $r_1\cdots r_N$ and $r_1'\cdots r_N'$ every term is the same, and in the term with permutation π, we can just relabel the summation variable $r'_{\pi(2)} \to r_2'$. Similarly, we can relabel r_i to be r_1 and r_j' to be r_1'. Actually, it's better to do it in the other order: first relabel r_i

to be r_1 and r'_j to be r'_1. This gives

$$\left\langle \psi^\dagger(r)\psi(r')\right\rangle = \sum_{r_2\cdots r_N}\sum_{r'_2\cdots r'_N} \underbrace{\Psi^\star(r_i\cdots r\cdots r_N)\Psi(r'_j\cdots r'\cdots r'_N)}_{\Psi^\star(r_1\cdots r_N)\Psi(r'_1\cdots r'_N)\zeta^{i+j}} \frac{1}{N}\sum_{i,j}\zeta^{i+j}$$

$$\cdot \frac{1}{(N-1)!}\sum_\pi \zeta^\pi \delta^d(r_2 - r'_{\pi(2)})\cdots\delta^d(r_N - r'_{\pi(N)})$$

$$= \sum_{r_2\cdots r_N}\sum_{r'_2\cdots r'_N} \Psi^\star(r_1\cdots r_N)\Psi(r'_1\cdots r'_N)\underbrace{\frac{1}{N}\sum_{ij}\zeta^{2(i+j)}}_{=N}$$

$$\cdot \frac{1}{(N-1)!}\sum_\pi \zeta^\pi \delta^d(r_2 - r'_{\pi(2)})\cdots\delta^d(r_N - r'_{\pi(N)}) .$$

(In the first line r is in the ith place and r' is in the jth place.) Now in the term permuted by π, relabel $r'_i \to r'_{\pi(i)}$ and use $\frac{1}{(N-1)!}\sum_{\pi\in S_{N-1}} = 1$ to get

$$\left\langle \psi^\dagger(r)\psi(r')\right\rangle = N\sum_{r_2\cdots r_N}\Psi^\star(r, r_2\cdots r_N)\Psi(r', r_2\cdots r_N).$$

(b) [Bonus question] Prove that for a fermionic state the eigenvalues of $\rho_1(r, r')$ are between 0 and 1.

[Hint: for fermions, the expectation value of the number operator $\psi^\dagger(r)\psi(r)$ in any state is ≤ 1.]

4. **A charged particle, classically.** [If you did this problem earlier this quarter, please submit your solution again for bookkeeping purposes.] This problem is an exercise in calculus of variations, as well as an important ingredient in our discussion of particles in electromagnetic fields.

Consider the following action functional for a particle in three dimensions:

$$S[x] = \int dt\ \left(\frac{m}{2}\dot{\vec{x}}^2 - e\Phi(\vec{x}) + \frac{e}{c}\dot{\vec{x}}\cdot\vec{A}(x)\right) .$$

(a) Show that the extremization of this functional gives the equation of motion:

$$\frac{\delta S[x]}{\delta x^i(t)} = -m\ddot{x}^i(t) - e\partial_{x^i}\Phi(x(t)) + \frac{e}{c}\dot{x}^j F_{ij}(x(t))$$

where $F_{ij} \equiv \partial_{x^i}A_j - \partial_{x^j}A_i$. Show that this is the same as the usual Coulomb-Lorentz force law

$$\vec{F} = e\left(\vec{E} + \frac{\vec{v}}{c}\times\vec{B}\right)$$

with $B_i \equiv \frac{1}{2}\epsilon_{ijk}F_{jk}$.

(b) Show that the canonical momenta are

$$\Pi_i \equiv \frac{\partial L}{\partial \dot{x}^i} = m\dot{x}^i + \frac{e}{c}A_i(x).$$

Here $S = \int dtL$. (I call them Π rather than p to emphasize the difference from the 'mechanical momentum' $m\dot{x}$.) Show that the resulting Hamiltonian is

$$H \equiv \sum_i \dot{x}^i \Pi^i - L = \frac{1}{2m}\left(\Pi_i - \frac{e}{c}A_i(x(t))\right)^2 + e\Phi.$$