P3317 HW from Lecture 24+25 and Recitation 13

Due Nov 27, 2018

Problem 1. The Higgs Mechanism in 1+1 dimensional Quantum Electrodynamics
In lecture we explicitly went through a calculation of the Higgs mechanism for 2+1 dimensional scalar quantum electrodynamics. Recall the Higgs mechanism describes the physics of a gauge field coupled to a "Higgs" field. When the Higgs field acquires a finite mean value, the gauge modes become gapped. This is the model used to explain the masses of the W and Z bosons in the theory of the weak interactions. Here I will have you go through the same argument in 1+1 dimension.

We will use x to label the spatial dimension, and t the time dimension. We have one scalar field $\phi(x,t)$, the Higgs field. We will have two gauge fields: A_t and A_x. In one spatial dimension there is no analog of a magnetic field, but you can have an electric field. It is defined by

$$E = \partial_t A_x - \partial_x A_t. \tag{1}$$

In lecture we used the symbol S_y for this quantity.

We will start with the simplest case where the Higgs field obeys a relativistic wave equation

$$(\partial_t - iA_t)^2\phi - (\partial_x - iA_x)^2\phi + m^2\phi = 0. \tag{2}$$

The gauge fields obey "Maxwell" equations

$$\begin{aligned} \partial_x E + \frac{1}{2}\left[i\phi^*(\partial_t - iA_t)\phi - i\phi(\partial_t + iA_t)\phi^*\right] &= 0 \qquad (3)\\ -\partial_t E - \frac{1}{2}\left[i\phi^*(\partial_x - iA_x)\phi - i\phi(\partial_x + iA_x)\phi^*\right] &= 0 \end{aligned}$$

1.1. Show that these three equations [Eqs. (2)-(15)] possess a Gauge symmetry. That is they are invariant under the transformation

$$\begin{aligned} A_x &\to A_x + \partial_x\Lambda \qquad (4)\\ A_t &\to A_t + \partial_t\Lambda \qquad (5)\\ \phi &\to e^{i\Lambda}\phi. \qquad (6) \end{aligned}$$

Hint: First show that

$$(\partial_t - i(A_t + \partial_t\Lambda))e^{i\Lambda}\phi = e^{i\Lambda}(\partial_t - iA_t)\phi.$$

Next define $\psi = (\partial_t - iA_t)\phi$, and reuse your first result:

$$(\partial_t - i(A_t + \partial_t\Lambda))e^{i\Lambda}\psi = e^{i\Lambda}(\partial_t - iA_t)\psi.$$

Finally, putting these together yields

$$(\partial_t - i(A_t + \partial_t\Lambda))^2 e^{i\Lambda}\phi = e^{i\Lambda}(\partial_t - iA_t)^2\phi.$$

With these identities (and the similar ones for ∂_x) the arguments are straightforward.

Solution 1.1 (4 points)**.** Following the hint, we look at how the covarient derivative behaves under a gauge transform.

$$(\partial_t - i(A_t + \partial_t \Lambda))\, e^{i\Lambda}\phi = e^{i\Lambda}\left(\partial_t - iA_t - i\partial_t\Lambda\right)\phi + \left(\partial_t e^{i\Lambda}\right)\phi \tag{7}$$

$$= e^{i\Lambda}\left(\partial_t - iA_t - i\partial_t\Lambda + i\partial_t\Lambda\right)\phi \tag{8}$$

$$= e^{i\Lambda}\left(\partial_t - iA_t\right)\phi. \tag{9}$$

Typographically replacing t with x yields.

$$\left(\partial_x - iA_x\right)\phi \overset{\Lambda}{=} e^{i\Lambda}\left(\partial_x - iA_x\right)\phi. \tag{10}$$

We can then apply this twice to get

$$\left(\partial_t - iA_t - i\partial_t\Lambda\right)\left[\left(\partial_t - iA_t - i\partial_t\Lambda\right)e^{i\Lambda}\phi\right] = \left(\partial_t - iA_t - i\partial_t\Lambda\right)\left[e^{i\Lambda}\left(\partial_t - iA_t\right)\phi\right] \tag{11}$$

$$= e^{i\Lambda}\left(\partial_t - iA_t\right)\left[\left(\partial_t - iA_t\right)\phi\right]. \tag{12}$$

Thus if ϕ obeys Eq. (2), then for any arbitrary $\Lambda(x,t)$, one has $e^{i\Lambda}\phi$ obeys

$$(\partial_t - i(A_t + \partial_t\Lambda_{)}^{2} e^{i\Lambda}\phi - (\partial_x - i(A_x + \partial_x\Lambda)^2 e^{i\Lambda}\phi + m^2 e^{i\Lambda}\phi = 0. \tag{13}$$

Finally, in principle we should show that the electric field is invarient under the gauge transformation.

$$\partial_t A_x - \partial_x A_t \to \partial_t A_x + \partial_t\partial_x\Lambda - \partial_x A_t - \partial_x\partial_t\Lambda \tag{14}$$

$$= \partial_t A_x - \partial_x A_t$$

Thus Eq. (15) implies

$$\partial_x E + \frac{1}{2}\left[ie^{-i\Lambda}\phi^*(\partial_t - i(A_t + \partial_t\Lambda))e^{i\Lambda}\phi - ie^{i\Lambda}\phi(\partial_t + i(A_t + \partial_t\Lambda)e^{-i\Lambda}\phi^*\right] = 0 \tag{15}$$

$$-\partial_t E - \frac{1}{2}\left[ie^{-i\Lambda}\phi^*(\partial_x - i(A_x + \partial_x\Lambda))e^{i\Lambda}\phi - ie^{i\Lambda}\phi(\partial_x + i(A_x + \partial_x\Lambda))e^{-i\Lambda}\phi^*\right] = 0,$$

which expresses the desired symmetry.

Aside: a neat trick

A clever way to write this (which was very briefly mentioned in class, and is implicit in the hint) is:

$$D_t \to e^{i\Lambda} D_t e^{-i\Lambda} \tag{16}$$

such that:

$$D_t\phi \to e^{i\Lambda} D_t e^{-i\Lambda} e^{i\Lambda}\phi = e^{i\Lambda} D_t\phi \tag{17}$$

$$D_t^2\phi \to e^{i\Lambda} D_t e^{-i\Lambda} e^{i\Lambda} D_t e^{-i\Lambda} e^{i\Lambda}\phi = e^{i\Lambda} D_t^2\phi \tag{18}$$

and similarly for the x component. This is why $D_t \equiv (\partial_t - iA_t)$ is called a 'covariant derivative': $D_t\phi$ transforms in the same way as ϕ does under a gauge transformation, while the standard derivative $\partial_t\phi$ does not. The covariant derivative is many ways a simpler object than an ordinary derivative.

1.2. Linearize Eq. (2) about $\phi = A_x = A_t = 0$.

Solution 1.2 (2 points)**.** The linearized equations are:

$$(\partial_t^2 - \partial_x^2 + m^2)\phi = 0 \tag{19}$$

$$\partial_x E = 0 \tag{20}$$

$$\partial_t E = 0 \tag{21}$$

The last two equations[a] describe a constant electric field (in free space), and the first is a wave equation for ϕ with a mass term. Note that they are completely decoupled, and so we can solve them seperately.

[a]These are the 1+1 dimensional versions of Coulomb's and Faraday's laws in free space

1.3. Find the normal modes of this linearized equations. IE. Write $\phi(x,t) = \phi e^{ikx - i\omega t}$, and find what ω is allowed for a given k. How many independent modes do we have at each k? These correspond to particles and antiparticles (like electrons and positrons – but here they are bosonic).

As a side note, ϕ is a complex valued field so for fixed k_0, ω_0, each of the following complex exponentials are independent: $e^{i(k_0x-\omega_0t)}, e^{i(k_0x+\omega_0t)}, e^{i(-k_0x+omega_0t)}, e^{i(-k_0x-\omega_0t)}$. If ϕ was real valued things would be different: $\mathrm{re}(e^{i(k_0x-\omega_0t)}) = \mathrm{re}(e^{i(-k_0x+\omega_0t)})$.

Solution 1.3 (2 points)**.** Making the subsitution $\phi(x,t) = \phi e^{ikx-i\omega t}$, we get:

$$\left(-\omega^2 + k^2 + m^2\right)\phi e^{ikx-i\omega t} = 0. \tag{22}$$

This is solved for:

$$\omega^2 = k^2 + m^2. \tag{23}$$

Since ϕ is a complex field, it has one complex degree of freedom, which is two real degrees of freedom (independent modes) for each k. That is, $\mathrm{Re}(\phi)$ and $\mathrm{Im}(\phi)$ are independent modes. Equivalently, the positive and negative frequency solutions to the above equation can be regarded as the two independent modes.

1.4. Write the "Maxwell" equations Eq. 15 in terms of the gauge fields.

Solution 1.4 (2 points)**.** Maxwell's equations can be written:

$$\partial_x\partial_t A_x - \partial_x^2 A_t + \frac{1}{2}\left[i\phi^*\left(\partial_t - iA_t\right)\phi - i\phi\left(\partial_t + iA_t\right)\phi^*\right] = 0 \tag{24}$$

$$-\partial_t\partial_x A_t + \partial_t^2 A_x - \frac{1}{2}\left[i\phi^*\left(\partial_x - iA_x\right)\phi - i\phi\left(\partial_x + iA_x\right)\phi^*\right] = 0 \tag{25}$$

1.5. Linearize these equations about $\phi = A_x = A_t = 0$.

Solution 1.5 (2 points)**.** Linearized about $\phi = A_x = A_t = 0$ leaves just the free-space Maxwell's equations:

$$\partial_x \partial_t A_x - \partial_x^2 A_t = 0 \tag{26}$$

$$\partial_t \partial_x A_t - \partial_t^2 A_x = 0 \tag{27}$$

1.6. Write $A_t(x,t) = A_t e^{ikx - i\omega t}$ and $A_x(x,t) = A_x e^{ikx-i\omega t}$. Substitute these into the linearized equations to find a matrix equation

$$\begin{pmatrix} ? & ? \\ ? & ? \end{pmatrix} \begin{pmatrix} A_x \\ A_t \end{pmatrix} = 0. \tag{28}$$

Rearrange the equations so that the matrix is symmetric.

Solution 1.6 (3 points)**.** These equations can be written:

$$\begin{pmatrix} -\partial_x^2 & \partial_x \partial_t \\ \partial_t \partial_x & -\partial_t^2 \end{pmatrix} \begin{pmatrix} A_t \\ A_x \end{pmatrix} = 0. \tag{29}$$

Substrituting in $A_{x,y} = e^{ikx-i\omega t} A_{x,y}$ gives:

$$\begin{pmatrix} k^2 & \omega k \\ \omega k & \omega^2 \end{pmatrix} \begin{pmatrix} A_t \\ A_x \end{pmatrix} = 0. \tag{30}$$

We write this as a symmetric matrix because we want to turn the problem of simultaneous equations into an eigenvalue problem. In particular, we want to decompose some arbitrary vector of A_t, A_x in to eigenvectors of the matrix above. If we can make such a decomposition, then the equation above is equivalent as saying that the corresponding eigenvalues are zero. Symmetric eigenvalue problems are easier to solve.

1.7. Find the eigenvalues and eigenvectors of this matrix. You should find one vector where the eigenvalue is always zero, and another where the eigenvalue is never zero.

Solution 1.7 (3 points)**.** There is an eigenvector:

$$N \begin{pmatrix} \omega & -k \end{pmatrix}^T \tag{31}$$

with eigenvalue 0, and an eigenvector

$$N \begin{pmatrix} k & \omega \end{pmatrix}^T \tag{32}$$

with eigenvalue $k^2 + \omega^2$. Note that there is no non-trivial solution to the equation $k^2 + \omega^2 = 0$ for real ω, k.

1.8. What is the physical significance of the eigenvector with zero eigenvalue? What is the electric field E for this mode? [E is the only physical field – there is no magnetic field in 1D.]

Solution 1.8 (3 points)**.** The eigenvector with zero eigenvalue corresponds to an E field given by:

$$E = N\left(-k\partial_t e^{ikx-i\omega t} - \omega\partial_x e^{ikx-i\omega t}\right) = iNe^{ikx-i\omega t}\left(k\omega - \omega k\right) = 0. \tag{33}$$

That is, this mode has no physical significance, it is 'pure gauge' and does not contribute to any observable dynamics. 'Pure gauge' means that it is a gauge transformation of $A_t = A_x = 0$. Clearly this particular choice of gauge field does not correspond to a physical travelling wave. Alternatively, consider a gauge transformation with parameter $\Lambda = e^{ikx-i\omega t}$:

$$\begin{pmatrix} A_t \\ A_x \end{pmatrix} = \begin{pmatrix} 0 + \partial_t e^{ikx-i\omega t} \\ 0 + \partial_x e^{ikx-i\omega t} \end{pmatrix} = -i\begin{pmatrix} \omega \\ -k \end{pmatrix} e^{ikx-i\omega t}. \tag{34}$$

We therefore see that this mode is just a gauge transformation on $A = 0$.

1.9. In 3D we have 2 propegating modes for each k – these are the two transverse polarizations of the photon. In 2D we only found one – there is only one transverse direction. How many photon modes do we find in this 1D model?

Solution 1.9 (1 point)**.** In 1D, there are no transverse directions. There are no possible polarizations for the photon. There therefore cannot be any physical modes associated with the photon. This is indeed what we found, when we showed that there are no real solutions to the equations of motion of the electromagnetic potentials with the form of a wave.

Now that we understand this simple model, we are ready to study a less trivial model which illustrates the Higgs mechanism. Lets replace Eq. (2) with

$$(\partial_t - iA_t)^2\phi - (\partial_x - iA_x)^2\phi - m^2\phi + \lambda^2|\phi|^2\phi = 0. \tag{35}$$

1.10. Now linearize the Higgs equation Eq. (35) about $\phi_0 = m/\lambda$, and about $A_x, A_t = 0$. [Write $\phi = \phi_0 + a + ib$.] Take the real and imaginary parts of the equation for ϕ, so that you have two real equations. Note: you must do this separation into real and imaginary parts now, before question 1.11 where you take the Fourier transform. You will get the wrong answer if you take the Fourier transform first.

Solution 1.10 (4 points)**.** Let's go term by term. The first term becomes

$$(\partial_t - iA_t)^2 (\phi_0 + a + ib) = \partial_t^2 a + i\partial_t^2 b - i\phi_0 \partial_t A_t + ... \tag{36}$$

where the ... corresponds to quadratic and higher order terms. Similarly for the second term:

$$-(\partial_x - iA_x)^2 (\phi_0 + a + ib) = -\partial_x^2 a - i\partial_x^2 b + i\phi_0 \partial_x A_x + ... \tag{37}$$

The third term is simply:

$$-m^2 (\phi_0 + a + ib) = -m^2\phi_0 - m^2 a - im^2 b, \tag{38}$$

and the final term:

$$\lambda^2 |\phi_0 + a + ib|^2 (\phi_0 + a + ib) = \lambda^2\phi_0^3 + 3\lambda^2\phi_0^2 a + i\lambda^2\phi_0^2 b + ... \tag{39}$$

Putting them all together gives:

$$\partial_t^2 a + i\partial_t^2 b - i\phi_0\partial_t A_t - \partial_x^2 a - i\partial_x^2 b + i\phi_0\partial_x A_x + 2m^2 a = 0 \tag{40}$$

where some terms cancelled due to the value of ϕ_0. Taking the real and imaginary parts gives:

$$\left(\partial_t^2 - \partial_x^2 + 2m^2\right) a = 0 \tag{41}$$
$$\left(\partial_t^2 - \partial_x^2\right) b + \phi_0 \left(\partial_x A_x - \partial_t A_t\right) = 0 \tag{42}$$

1.11. Write $a(x,t) = ae^{ikx-i\omega t}$, $b(x,t) = be^{ikx-i\omega t}$, $A_t(x,t) = A_t e^{ikx-i\omega t}$ and $A_x(x,t) = A_x e^{ikx-i\omega t}$. Substitute these into the linearized Higgs equation. One equation should decouple, the other will connect b, A_t and A_x.

Solution 1.11 (2 points)**.** Making the given substitutions, we get:

$$a\left(\partial_t^2 - \partial_x^2 + 2m^2\right) e^{ikx-i\omega t} = 0 \tag{43}$$
$$b\left(\partial_t^2 - \partial_x^2\right) e^{ikx-i\omega t} + \phi_0 \left(A_x\partial_x - A_t\partial_t\right) e^{ikx-i\omega t} = 0 \tag{44}$$

$$\implies a\left(\omega_a^2 - k_a^2 - 2m^2\right) = 0 \tag{45}$$
$$b\left(-\omega^2 + k^2\right) + i\phi_0 \left(A_x k + A_t\omega\right) = 0 \tag{46}$$

1.12. Linearize the Maxwell equations about $\phi_0 = m/\lambda$, and about $A_x, A_t = 0$.

Solution 1.12 (3 points)**.** First let's linearize just one term:

$$i\phi^*\left(\partial_t - iA_t\right)\phi = i\left(\phi_0 + a + ib\right)^*\left(\partial_t - iA_t\right)\left(\phi_0 + a + ib\right) \tag{47}$$
$$= \phi_0^2 A_t - \phi_0 \partial_t b + i\phi_0 \partial_t a + ... \tag{48}$$

The expressions for the other terms are very similar:

$$-i\phi\left(\partial_t + iA_t\right)\phi^* = \phi_0^2 A_t - \phi_0 \partial_t b - i\phi_0 \partial_t a + ... \tag{49}$$
$$i\phi^*\left(\partial_x - iA_x\right)\phi = \phi_0^2 A_x - \phi_0 \partial_x b + i\phi_0 \partial_x a + ... \tag{50}$$
$$-i\phi\left(\partial_x + iA_x\right)\phi^* = \phi_0^2 A_x - \phi_0 \partial_x b - i\phi_0 \partial_x a + ... \tag{51}$$

Putting these expressions together into Maxwells equations gives the linearized form:

$$\partial_x \partial_t A_x - \partial_x^2 A_t + \phi_0^2 A_t - \phi_0 \partial_t b = 0 \tag{52}$$
$$\partial_t \partial_x A_t - \partial_t^2 A_x - \phi_0^2 A_x + \phi_0 \partial_x b = 0 \tag{53}$$

1.13. Write $a(x,t) = ae^{ikx - i\omega t}$, $b(x,t) = be^{ikx-i\omega t}$, $A_t(x,t) = A_t e^{ikx-i\omega t}$ and $A_x(x,t) = A_x e^{ikx-i\omega t}$. Substitute these into the linearized Higgs equation.

Solution 1.13 (2 points)**.** Substituting in the wave ansatz gives:

$$\left(A_x \partial_x \partial_t - A_t \partial_x^2 + \phi_0^2 A_t - \phi_0 b \partial_t\right) e^{ikx-i\omega t} = 0 \tag{54}$$
$$\left(A_t \partial_t \partial_x - A_x \partial_t^2 - \phi_0^2 A_x + \phi_0 b \partial_x\right) e^{ikx-i\omega t} = 0 \tag{55}$$

and so

$$\omega k A_x + \left(k^2 + \phi_0^2\right) A_t + i\omega\phi_0 b = 0 \tag{56}$$
$$\omega k A_t + \left(\omega^2 - \phi_0^2\right) A_x + ik\phi_0 b = 0 \tag{57}$$

1.14. Combine the results of problem 1.11 and 1.13 as a matrix equation

$$\begin{pmatrix} ? & ? & ? \\ ? & ? & ? \\ ? & ? & ? \end{pmatrix} \begin{pmatrix} A_x \\ A_t \\ b \end{pmatrix} = 0. \tag{58}$$

Rearrange things so that this matrix is Hermitian.

Solution 1.14 (3 points)**.** These can be summarized in the matrix equation:

$$\begin{pmatrix} \omega^2 - \phi_0^2 & \omega k & ik\phi_0 \\ \omega k & k^2 + \phi_0^2 & i\omega\phi_0 \\ ik\phi_0 & i\omega\phi_0 & k^2 - \omega^2 \end{pmatrix} \begin{pmatrix} A_x \\ A_t \\ b \end{pmatrix} = 0. \tag{59}$$

In order to get it in to the same form as in the lecture notes, we can multiply the equation coming from the last row of the matrix by an overall negative sign, which is just convention and doesn't change the physics:

$$\begin{pmatrix} \omega^2 - \phi_0^2 & \omega k & ik\phi_0 \\ \omega k & k^2 + \phi_0^2 & i\omega\phi_0 \\ -ik\phi_0 & -i\omega\phi_0 & \omega^2 - k^2 \end{pmatrix} \begin{pmatrix} A_x \\ A_t \\ b \end{pmatrix} = 0. \tag{60}$$

1.15. Find the eigenvalues and eigenvectors of this matrix. You should find one mode where the eigenvalue is always zero, one where the eigenvalue is never zero, and a third which has an eigenvalue which is zero when $\omega^2 = k^2 + \phi_0^2$. This last mode is the massive gauge boson (the analog of the W boson).

Solution 1.15 (3 points)**.** I used Mathematica to get the following eigenvectors and eigenvalues:

$$\begin{array}{ll} \text{Eigenvector} & \text{Eigenvalue} \\ \begin{pmatrix} ik, & -i\omega, & \phi \end{pmatrix} & 0 \\ \begin{pmatrix} ik\omega, & i(k^2+\phi_0^2), & \omega\phi_0 \end{pmatrix} & \omega^2 + k^2 + \phi_0^2 \\ \begin{pmatrix} -i\phi_0, & 0, & k \end{pmatrix} & \omega^2 - k^2 - \phi_0^2 \end{array} \tag{61}$$

where the eigenvectors are only defined up to normalization. As expected, one eigenvalue is always zero (and corresponds to a gauge transformation, one is never zero, and the last is the massive gauge field.

Problem 2. Mass of the Higgs boson

The mass of the W boson is $80GeV/c^2$.

2.1. Given our argument about the Higgs mechanism, can you say anything about the Higgs boson mass? [What is the expression for the mass of the gauge fields and the mass of the Higgs. Are there any free parameters?]

Hint: This is actually a trick question. The conventional wisdom is that you can't actually determine the mass of the Higgs from the mass of the W. Why is that so?

[Interestingly enough, the experimental mass of the Higgs is $125GeV/c^2$, which is in the same ballpark as the W mass – making one think there is actually a connection.]

Solution 2.1 (2 points)**.** The equation of motion for the Higgs ϕ had two parameters, λ and m, and in problem 1 we saw that the mass it gave to the photon in Higgsed QED is $m_\gamma = m/\lambda$. In the Standard Model, the W and Z bosons get their masses by a similar mechanism. This formula means that a measurement of the W boson mass only tells you the value of the ratio m/λ. The Higgs mass is given by $m_h = \sqrt{2}m$ (The Higgs is the particle a in Eq. 41), which remains a free parameter.

Problem 3. Linear Combination of Atomic Orbitals

One way of modeling electronic structure in crystals is to imagine that the wavefunction of an electron is made from a linear combination of the atomic orbitals on each of the nuclei making up the solid. The simplest such model is to just use one orbital on each nucleus.

If r_j are the locations of each of the nuclei, then the ansatz is

$$\psi(r) = \sum_j \psi_j \phi(r - r_j), \tag{62}$$

where ψ_j are just a bunch of numbers, and $\phi(r)$ is the wavefunction of an orbital for a nucleus at the origin. [For concreteness you can imagine that $\phi(r) \sim e^{-\alpha|r|}$ is something like the 1s orbital of hydrogen. Regardless, we will imagine that we know $\phi(r)$ from some other calculation.]

Treating ψ as a variational wavefunction, the energy is

$$\begin{aligned} E &= \frac{\int dr\, \psi^*(r) H \psi(r)}{\int dr\, \psi^*(r)\psi(r)} && (63) \\ &= \frac{\sum_{ij} H_{ij}\psi_i^*\psi_j}{\sum_{ij} \Lambda_{ij}\psi_i^*\psi_j} && (64) \end{aligned}$$

where

$$\begin{aligned} H_{ij} &= \int dr\, \phi^*(r - r_i) H \phi(r - r_j) && (65) \\ \Lambda_{ij} &= \int dr\, \phi^*(r - r_i)\phi(r - r_j) && (66) \end{aligned}$$

3.1. Prove that H_{ij} depend on i and j only through the displacement $r_i - r_j$. Similarly, prove that Λ_{ij} also only depends on $r_i - r_j$.

Solution 3.1 (4 points)**.**

$$
\begin{aligned}
H_{ij} &= \int_{-\infty}^{\infty} dr\psi(r-r_i)H\psi(r-r_j) \\
&= \int_{-\infty}^{\infty} dr\psi(r-r_i)\left(-\frac{1}{2m}\frac{\partial^2}{\partial r^2}+V(r)\right)\psi(r-r_j) \\
&= \int_{-\infty}^{\infty} d(r'+r_i)\psi(r')\left(-\frac{1}{2m}\frac{\partial^2}{\partial(r'+r_i)^2}+V(r'+r_i)\right)\psi(r'+r_i-r_j) \\
&= \int_{-\infty-r_i}^{\infty-r_i} dr'\psi(r')\left(-\frac{1}{2m}\frac{\partial^2}{\partial r'^2}+V(r')\right)\psi(r'+r_i-r_j) \\
&= \int_{-\infty}^{\infty} dr\psi(r)\left(-\frac{1}{2m}\frac{\partial^2}{\partial r^2}+V(r)\right)\psi(r+r_i-r_j)
\end{aligned}
\tag{67}
$$

In the third line, we introduced a change of variables $r' = r - r_i$. In the fourth line, we used the fact that $V(r)$ is periodic, so $V(r') = V(r' + r_i)$. In the last line, we renamed the dummy variable r' back to r.

Similarly,

$$
\begin{aligned}
\Lambda_{ij} &= \int_{-\infty}^{\infty} dr\psi(r-r_i)\psi(r-r_j) \\
&= \int_{-\infty}^{\infty} d(r'+r_i)\psi(r')\psi(r'+r_i-r_j) \\
&= \int_{-\infty-r_i}^{\infty-r_i} dr'\psi(r')\psi(r'+r_i-r_j) \\
&= \int_{-\infty}^{\infty} dr\psi(r)\psi(r+r_i-r_j)
\end{aligned}
\tag{68}
$$

We see that both H_{ij} and Λ_{ij} contains only the combination $r_i - r_j$.

3.2. What happens to H_{ij} and Λ_{ij} l when r_i and r_j are far apart?

Solution 3.2 (1 point)**.** If r_i and r_j are very far apart, the overlap between the wavefunctions $\phi(r - r_i)$ and $\phi(r - r_j)$, and hence H_{ij} and Λ_{ij}, becomes very small.

To leading order we only need to keep diagonal terms, and terms where the two atoms are nearest neighbors:

$$
H_{ij} \approx \begin{cases} E_0 & i = j \\ -\Delta & i, j \text{ are neighbors} \\ 0 & \text{otherwise} \end{cases} \tag{69}
$$

$$
\Lambda_{ij} \approx \begin{cases} 1 & i = j \\ \epsilon & i, j \text{ are neighbors} \\ 0 & \text{otherwise} \end{cases} \tag{70}
$$

Expanding to first order in the small parameters ϵ and Δ, we have

$$\begin{aligned} E &= \frac{E_0 \sum_i \psi_i^* \psi_i - t \sum_{\langle i,j \rangle} (\psi_i^* \psi_j + \psi_j^* \psi_i)}{\sum_i \psi_i^* \psi} && (71) \\ t &= \epsilon E_0 + \Delta, && (72) \end{aligned}$$

where the $\langle i,j \rangle$ indicates that we only sum over nearest neighbor pairs. Specializing to one dimension, this is

$$E = \frac{E_0 \sum_i \psi_i^* \psi_i - t \sum_i \left(\psi_{i+1}^* \psi_i + \psi_i^* \psi_{i+1} \right)}{\sum_i \psi_i^* \psi_i}. \quad (73)$$

To optimize this wavefunction, we want to set

$$\frac{\partial E}{\partial \psi_j^*} = 0. \quad (74)$$

Note that this is just a regular partial derivative: ψ_j^* is just an ordinary variable like x.

3.3. Prove that

$$\frac{\partial E}{\partial \psi_j^*} = \frac{-A\psi_{j+1} - A\psi_{j-1} + (E_0 - E)\psi_j}{\sum_i \psi_i^* \psi_i}, \quad (75)$$

and find A. [You may find it useful to look back at the lecture notes on the "Variational Principle" lecture, and on the "Hartree" lecture, both of which took similar derivatives.]

Solution 3.3 (3 points)**.** Some useful results:

$$\begin{aligned} \frac{\partial}{\partial \psi_j^*} \left(\sum_i \psi_i^* \psi_i \right) &= \sum_i \delta_{i,j} \psi_i = \psi_j \\ \frac{\partial}{\partial \psi_j^*} \left(\sum_i \psi_{i+1}^* \psi_i \right) &= \sum_i \delta_{i+1,j} \psi_i = \sum_i \delta_{i,j-1} \psi_i = \psi_{j-1} \\ \frac{\partial}{\partial \psi_j^*} \left(\sum_i \psi_i^* \psi_{i+1} \right) &= \sum_i \delta_{i,j} \psi_{i+1} = \psi_{j+1} \end{aligned} \quad (76)$$

Therefore, we find that

$$\begin{aligned} \frac{\partial E}{\partial \psi_j^*} &= \frac{\frac{\partial \left(E_0 \sum_i \psi_i^* \psi_i - t \sum_i (\psi_{i+1}^* \psi_i + \psi_i^* \psi_{i+1}) \right)}{\partial \psi_j^*}}{\sum_i \psi_i^* \psi_i} - \frac{\left(E_0 \sum_i \psi_i^* \psi_i - t \sum_i (\psi_{i+1}^* \psi_i + \psi_i^* \psi_{i+1}) \right) \frac{\partial (\sum_i \psi_i^* \psi_i)}{\partial \psi_j^*}}{\left(\sum_i \psi_i^* \psi_i \right)^2} \\ &= \frac{E_0 \psi_j - t(\psi_{j-1} + \psi_{j+1})}{\sum_i \psi_i^* \psi_i} - \frac{\left(E_0 \sum_i \psi_i^* \psi_i - t \sum_i (\psi_{i+1}^* \psi_i + \psi_i^* \psi_{i+1}) \right) \psi_j}{\left(\sum_i \psi_i^* \psi_i \right)^2} \\ &= \frac{-t(\psi_{j-1} + \psi_{j+1})}{\sum_i \psi_i^* \psi_i} + \frac{(E_0 - E)\psi_j}{\sum_i \psi_i^* \psi_i} \\ &= \frac{-t\psi_{j+1} - t\psi_{j-1} + (E_0 - E)\psi_j}{\sum_i \psi_i^* \psi_i} \end{aligned} \quad (77)$$

Hence we see that $A = t$.

Setting this expression equal to zero, we are left with the eigenvalue problem

$$-A\psi_{j+1} - A\psi_{j-1} + E_0\psi_j = E\psi_j, \tag{78}$$

which is the same form as our finite difference approximation to the Schrodinger equation.

3.4. We can solve this infinite set of equations with the following ansatz:

$$\psi_j = \alpha e^{ikaj} \tag{79}$$

where a is the spacing between the nuclei, k is a parameter, and α is chosen for normalization. Plugging this ansatz into Eq. (78), find a relationship between E and k. Leave your answer in terms of A.

Solution 3.4 (3 points)**.** Plugging in the ansatz, we have

$$\begin{aligned} \alpha\left(-Ae^{ika(j+1)} - Ae^{ika(j-1)} + E_0e^{ikaj}\right) &= \alpha\left(-2Ae^{ikaj}\cos(ka) + E_0e^{ikaj}\right) \\ &= \alpha Ee^{ikaj} \end{aligned} \tag{80}$$

Dividing by common factors on both sides, this reduce to the relation

$$E = E_0 - 2A\cos(ka) \tag{81}$$

Problem 4. Feedback

4.1. How long did this homework take?

4.2. Which of the following words come to mind when you think about this homework (feel free to add your own words if you have something better): frustrating, fun, tedious, insightful, hard, easy, useful, useless, fair, unfair