P3317 HW from Lecture 26+27 (HW 14)

Due Dec 4, 2018

Problem 1. Band Stucture of Sinusoidal Lattice
Here we will calculate the Band Structure from a sinusoidal potential. Such potentials arise in modeling cold atoms trapped in standing waves of light (so-called optical lattices). In dimensionless coordinates, the time independent Schrodinger equation would read:

$$E\psi = -\frac{1}{2}\partial_y^2\psi + U\cos(2\pi y)\psi. \tag{1}$$

Here $y = x/a$, $U = (ma^2/\hbar^2)V_0$ and $E = (ma^2/\hbar^2)\mathcal{E}$, where a is the lattice spacing $\mathcal{E}$ is the energy, m is the atomic mass, and V_0 is the "lattice depth". A typical cold atom experiment will have $a = 700$nm, and $m = 87$ times the proton mass. The depth U can vary from 0 to 50.

By Bloch's theorem, we can write the wavefunction as a plane wave times a periodic function,

$$\psi(y) = e^{iky}u(y), \tag{2}$$

where $u(y)$ is a periodic function, $u(y+1) = u(y)$. We can write $u(y)$ as a Fourier series, leading to the Ansatz:

$$\psi(y) = e^{iky}\sum_n e^{2\pi iny}u_n. \tag{3}$$

1.1. Substitute the ansatz in Eq. (3) into the Schrodinger equation, Eq. (1), to produce an equation of the form

$$\sum_n Ee^{iky}u_n e^{2\pi iny} = \sum_n A_n e^{iky}e^{2\pi iny}u_n + \sum_n B_n e^{iky}e^{2\pi i(n+1)y}u_n + \sum_n C_n e^{iky}e^{2\pi i(n-1)y}u_n, \tag{4}$$

where A_n, B_n, C_n do not depend on y. Find A_n, B_n, C_n.

Solution 1.1 (2 points)**.** Noting that $\cos(x) = (e^{ix} + e^{-ix})/2$, we see that

$$A_n = \frac{(ky + 2\pi n)^2}{2} \tag{5}$$

$$B_n = \frac{U}{2} \tag{6}$$

$$C_n = \frac{U}{2}. \tag{7}$$

1.2. Shift the dummy index n in some of the terms in Eq. (4) to make an equation in which the y dependence of each term is of the form $\exp(iky + 2\pi iny)$. Leave your answer in terms of A_n, B_n, C_n – do not substitute in your expressions for these.

Solution 1.2 (2 points)**.** No changes need to be made for the left hand side. On the right hand side, we leave the A term alone, shift $n \to n-1$ in the B term, and $n \to n+1$ in the C term to get:

$$\sum_n Ee^{iky}u_n e^{2\pi iny} = \sum_n A_n e^{iky}e^{2\pi iny}u_n + \sum_n B_{n-1}e^{iky}e^{2\pi iny}u_{n-1} + \sum_n C_{n+1}e^{iky}e^{2\pi iny}u_{n+1}. \quad (8)$$

1.3. Identifying the Fourier components on the left and right of your equation to generate a recursion relationship between u_n, u_{n+1}, and u_{n-1}. Show your work. Give your answer in terms of A_n, B_n, C_n – do not substitute in your expressions for these.

Solution 1.3 (2 points)**.**

$$Eu_n = A_n u_n + B_{n-1}u_{n-1} + C_{n+1}u_{n+1} \quad (9)$$

1.4. If you did everything right, your result from the last problem can be rewritten as

$$Eu_n = \frac{(k+2\pi n)^2}{2}u_n + \frac{U}{2}u_{n-1} + \frac{U}{2}u_{n+1}. \quad (10)$$

(You do not have to prove this). This can be thought of as a matrix equation.

In particular, we can truncate this to a $(2N+1) \times (2N+1)$ matrix equation by assuming that $u_n = 0$ unless $-N \le n \le N$.

Explicitly write the 5×5 matrix for the case $N = 2$.

Solution 1.4 (2 points)**.** For $N = 2$, the matrix should look like

$$\begin{pmatrix} \frac{(k-4\pi)^2}{2} & \frac{U}{2} & 0 & 0 & 0 \\ \frac{U}{2} & \frac{(k-2\pi)^2}{2} & \frac{U}{2} & 0 & 0 \\ 0 & \frac{U}{2} & \frac{k^2}{2} & \frac{U}{2} & 0 \\ 0 & 0 & \frac{U}{2} & \frac{(k+2\pi)^2}{2} & \frac{U}{2} \\ 0 & 0 & 0 & \frac{U}{2} & \frac{(k+4\pi)^2}{2} \end{pmatrix} \quad (11)$$

1.5. Write a computer program which given k and U generates this 5×5 matrix. Print out the matrix you find for $k = 0$ and $U = 5$. You do not need to include your code.

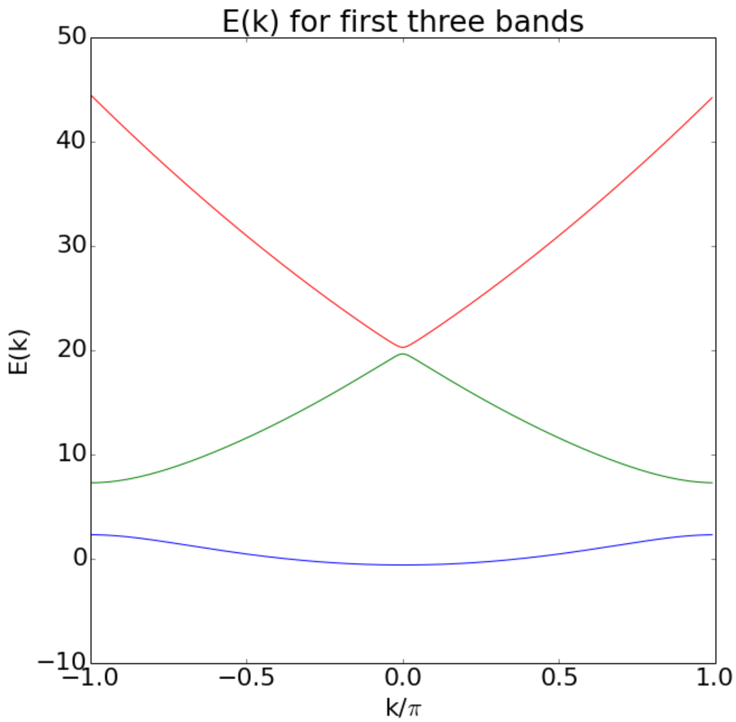
Solution 1.5 (2 points)**.** Plugging in $k = 0$, $U = 5$ gives

$$\begin{pmatrix} 78.95683521 & 2.5 & 0 & 0 & 0 \\ 2.5 & 19.7392088 & 2.5 & 0 & 0 \\ 0 & 2.5 & 0 & 2.5 & 0 \\ 0 & 0 & 2.5 & 19.7392088 & 2.5 \\ 0 & 0 & 0 & 2.5 & 78.95683521 \end{pmatrix} \quad (12)$$

1.6. Numerically find the 5 eigenvalues of that matrix [the one you get when $k = 0$ and $U = 5$]. (Again, no need to include your code.)

Solution 1.6 (2 points)**.** I found the following eigenvalues: -0.61645826, 19.63385334, 20.25003057, 79.0624717, 79.06219067

1.7. By looping over values of k from $-\pi$ to π, make a plot of $E(k)$ for the first 3 bands. As before, take $N = 2$, and $U = 5$. Be sure to label your axes. You do not need to include your code.



Solution 1.7 (5 points)**.**

1.8. In class we showed that a wavepacket centered around some k will have a velocity $v = \partial E/\partial k$. In our dimensionless variables, what is the maximum velocity of a particle in the lowest band for $U = 5$?

Solution 1.8 (2 points)**.** By numerically taking the derivative I found that in these dimensionless units the maximum velocity was roughly 1.5.

1.9. Use the parameters given above to convert your result to a velocity in m/s.

Solution 1.9 (2 points). Define $p = \hbar k/a$, and $\mathcal{E} = \frac{\hbar^2}{ma^2}E$. The dimensionful maximum group velocity is given by:

$$\begin{aligned} v_g &= \frac{\partial \mathcal{E}}{\partial p} \\ &= \frac{\hbar^2}{ma^2}\frac{a}{\hbar}\frac{\partial E}{\partial k} \\ &= \frac{\hbar}{ma} \times 1.50 \\ &= 0.00155\,\mathrm{m/s} \end{aligned} \tag{13}$$

Problem 2. Another approach to finding band structure is to work in real space instead of momentum space. We want to numerically solve the quantum mechanics problem

$$E\psi(x) = -\frac{\partial_x^2\psi(x)}{2m} + V(x)\psi(x) \tag{14}$$

where $V(x+a) = V(x)$. We want solutions of the form $\psi(x+a) = e^{ika}\psi(x)$. It clearly suffices to find $\psi(x)$ for $0 \le x \le a$

2.1. Write a finite difference approximation to this problem. [You don't need to do this on the computer, it suffices to just show the matrix on paper.] Explain how the boundary condition $\psi(x+a) = e^{ika}\psi(x)$ should appear in the matrix.

Solution 2.1 (5 points)**.** Let us start with $N+1$ grid points, so the grid spacing is $\delta = a/N$, and the grid points are at $x = \{0, \delta, 2\delta, ..., a-\delta, a\}$.
Let j be the grid index. We throw away the $(N+1)$th grid point $j = N$ at $x = a$ since it is related to the first grid point $j = 0$ at $x = 0$ by a phase, and hence should not be treated as a separate dynamical variable. So now j runs from 0 to $N-1$.
Define $x_j \equiv j\delta$, $\psi_j \equiv \psi(x_j)$ and $V_j \equiv V(x_j)$.

In the bulk of the grid, i.e. for $j = 1..N-2$, the finite difference version of Schrodinger's equation becomes

$$E\psi_j = -\frac{\psi_{j+1} + \psi_{j-1} - 2\psi_j}{2m\delta^2} + V_j\psi_j \tag{15}$$

What about $j = 0$ and $j = N-1$? Imposing the given boundary condition means that $\psi_{N-1} = e^{ika}\psi_{-1}$, $\psi_N = e^{ika}\psi_0$ and $\psi_{N+1} = e^{ika}\psi_1$. We then have

$$\begin{aligned} E\psi_0 &= -\frac{\psi_1 + e^{-ika}\psi_{N-1} - 2\psi_0}{2m\delta^2} + V_0\psi_0 \\ E\psi_{N-1} &= -\frac{e^{ika}\psi_0 + \psi_{N-2} - 2\psi_{N-1}}{2m\delta^2} + V_{N-1}\psi_{N-1} \end{aligned} \tag{16}$$

We can now represent Schrodinger's equation in matrix form:

$$E\begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ ... \\ \psi_{N-2} \\ \psi_{N-1} \end{pmatrix} = \begin{pmatrix} \frac{2}{2m\delta^2} + V_0 & -\frac{1}{2m\delta^2} & 0 & ... & 0 & -e^{-ika}\frac{1}{2m\delta^2} \\ -\frac{1}{2m\delta^2} & \frac{2}{2m\delta^2} + V_1 & -\frac{1}{2m\delta^2} & ... & 0 & 0 \\ 0 & -\frac{1}{2m\delta^2} & \frac{2}{2m\delta^2} + V_2 & ... & 0 & 0 \\ ... & ... & ... & ... & ... & ... \\ 0 & 0 & 0 & ... & \frac{2}{2m\delta^2} + V_{N-2} & -\frac{1}{2m\delta^2} \\ -e^{ika}\frac{1}{2m\delta^2} & 0 & 0 & ... & -\frac{1}{2m\delta^2} & \frac{2}{2m\delta^2} + V_{N-1} \end{pmatrix} \begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ ... \\ \psi_{N-2} \\ \psi_{N-1} \end{pmatrix} \tag{17}$$

Problem 3. Resistivity of a 1d Fermi gas

In class we gave a nice semiclassical argument for the resistivity of a metal that was based on scattering off of impurities. Here is a similar argument that is framed more in terms of phonons and relaxation times, that makes use of what we now know about band structure.

3.1. Equilibrium energy We first need to know how to describe equilibrium. In the previous problems we saw that we can label the single particle eigenstates of a single band by a quasimomentum k with $-\pi/a < k < \pi/a$, where a is the lattice spacing. For this problem we will approximate the energy of these modes by $\epsilon_k = -2t\cos(ka)$, where t is a parameter with units of energy.

If we imagine putting this system in a big box with periodic boundary conditions, we should further restrict $k = 2\pi n/L$, where $n = 0, \pm 1, \cdots$ is an integer. This leaves us with $N_L = L/a$ distinct values for k – one for each lattice site. We will assume $N_L \gg 1$.

Suppose we fill the lowest $N \gg 1$ states with one fermion in each (neglect spin). Clearly $0 \leq N \leq N_L$. Write a sum which corresponds to the total energy of the system. Approximate the sum as an integral, and calculate the ground state energy $\mathcal{E}$ as a function of N. You should find that the energy density $\mathcal{E}/L$ is only a function of the filling factor $\eta = N/N_L$, and the ratio t/a.

Solution 3.1 (3 points)**.** We note that since $-\pi/a < k < \pi/a$, E_k increases monotonically with increasing $|k|$, i.e. increasing $|n|$. Hence we can start filling up the energy levels in the order $n = 0, \{1, -1\}, \{2, -2\}, \ldots$

$$\mathcal{E} = \sum_{n=-N/2}^{N/2} (-2t)\cos(2\pi na/L) \tag{18}$$

To convert this into an integral, let us define the variable $x = 2\pi na/L$. x changes in steps of $2\pi a/L$, so we can think of $\delta x = 2\pi a/L$.

$$\begin{aligned}\mathcal{E} &= -2t\frac{L}{2\pi a}\int_{-2\pi(N/2)a/L}^{2\pi(N/2)a/L} dx\cos(x)\\ &= -\frac{Lt}{\pi a}\left[\sin(\pi Na/L) - \sin(-\pi Na/L)\right]\\ &= -\frac{2Lt}{\pi a}\sin(\pi\eta)\end{aligned} \tag{19}$$

3.2. Imagine that we give every electron a very small impulse p. One expects that the filled states will now be those with $-N/2 + pL/(2\pi) < n < N/2 + pL/(2\pi)$. Calculate the total current

$$j = \frac{q}{L}\sum_{k,\text{ occupied}} \frac{\partial \epsilon_k}{\partial k} \tag{20}$$

where the sum is over only the occupied states. The total current should be zero when the impulse is zero, and it should be intensive. That is, if we double the number of particles, and double the system size, we should find that j is unchanged. [As before, to calculate the sum, convert it into an integral.]

Solution 3.2 (3 points)**.**

$$\frac{\partial E_k}{\partial k} = 2ta\sin(ka) \tag{21}$$

Therefore,

$$\begin{aligned}j &= \frac{q}{L}\sum_{k,\text{occupied}} \frac{\partial E_k}{\partial k}\\ &= \frac{q}{L}2ta\sum_{n=-N/2+pL/(2\pi)}^{N/2+pL/(2\pi)} \sin(2\pi na/L)\\ &= \frac{q}{L}2ta\frac{L}{2\pi a}\int_{-\pi Na/L+pa}^{\pi Na/L+pa} dx\sin(x)\\ &= \frac{tq}{\pi}\left[-\cos(\pi Na/L + pa) + \cos(-\pi Na/L + pa)\right]\\ &= \frac{2tq}{\pi}\sin(\pi\eta)\sin(pa)\end{aligned} \tag{22}$$

3.3. For small p we can linearize the current, writing

$$j = \alpha p + \mathcal{O}(p^2). \tag{23}$$

Calculate α.

Solution 3.3 (2 points)**.**

$$\begin{aligned} j &= \frac{2tq}{\pi}\sin(\eta)\sin(pa) = \frac{2atq}{\pi}\sin(\eta)p + O(p^2) \\ \alpha &= \frac{2atq}{\pi}\sin(\pi\eta) \end{aligned} \tag{24}$$

3.4. We now model the interactions between the phonons and the electrons by a "mean free time". We apply an electric field of strength E, allowing the electrons to accelerate. After a time τ the electrons transfer their energy to phonons, and return to their ground state. The impulse during time τ is then $p = qE\tau$. The average current is then

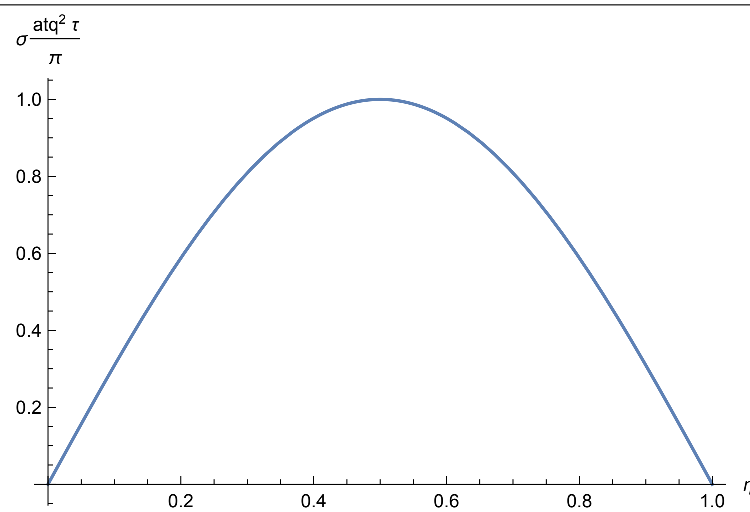
$$\bar{j} = \frac{\alpha q E \tau}{2}. \tag{25}$$

The factor of two arises because the velocity is rising linearly with time. We saw this same factor in lecture. Within this model, what is the conductivity σ_c in terms of α? After giving that result, substitute your expression for α from problem 3.3.

Solution 3.4 (1 point)**.**

$$\begin{aligned} \bar{j} = \sigma_c E &= \frac{\alpha q E \tau}{2} = \frac{2atq^2E\tau}{2\pi}\sin(\pi\eta) \\ \sigma_c &= \frac{atq^2\tau}{\pi}\sin(\pi\eta) \end{aligned} \tag{26}$$

3.5. Make a plot of the conductivity as a function of the filling $\eta = N/N_L$, with η running from 0 to 1. Label your axes.



Solution 3.5 (5 points)**.**

3.6. What is the conductivity when the band is either completely full or completely empty?

Solution 3.6 (1 point)**.** We see that the conductivity is zero when $\eta = 0$ or $\eta = 1$, i.e. when the band is completely empty or full.

Problem 4. The Meisner Effect

The Higgs mechanism (which was used in a previous lecture to explain the masses of the gauge bosons in the theory of the weak interaction) has connections to solid state physics.

Aluminum, when cooled to 1.2K, enters a state of zero resistivity, known as a superconductor. What is particularly unusual about this state is that it "expels" magnetic fields. For example imagine putting a chunk of aluminum in a solenoid. Cool it down to 1.2K. You will find that the magnetic field is zero in the aluminum – and a little bigger around it (to account for conservation of magnetic flux). There were a number of phenomonological descriptions of this, including one usually attributed to P. W. Anderson which is widely said to be the inspiration for the Higgs mechanism. [Certainly Anderson claims that it was.]

The basic physics of superconductivity is that there is a weak phonon-mediated interaction between electrons which allow them to form "Cooper pairs". These pairs are bosons, and at sufficiently low temperature they all occupy the same quantum state. The wavefunction of this state is then a macroscopic observable. In the appropriate regime, this wavefunction will obey the "time dependent Gizburg-Landau equation"

$$(i\partial_t - q\phi)\psi = -\frac{1}{2m}(\nabla - iq\mathbf{A})^2\psi - a^2\psi + b^2|\psi|^2\psi, \tag{27}$$

where $q = -2e$ is the charge of a pair, and $m = 2m_e$ is the mass of a pair. The constants a and b are phenomonological – but can be calculated for some simple models. This is simply a non-relativistic version of our scalar QED calculation from lecture 14. Physically a^2 represents the forces driving the system to form cooper pairs, it is positive in the "symmetry broken phase" $T < T_c$ and negative for $T > T_c$.

Having spent so much time doing the dynamics of a theory like this, you will not be surprised to find out that the photon modes inside a superconductor develop a gap. On physical grounds, this result should not be a surprise – how could light possibly propegate inside a superconductor? The electrons surely will screen out any electric field. Thus in this context the mysterious sounding "Higgs" mechanism is physically obvious. The resulting gapped mode is a "plasmon" – involving not only the gauge field, but also the motion of charges.

Rather than thinking about the dynamics, we can already see this physics from the static behavior, exploring the expelling of flux – the Meisner effect.

We will assume everything is static, and there are no electric fields. Further we will use a gauge where the scalar potential vanishes, $\phi = 0$, so that

$$-\frac{1}{2m}(\nabla - iq\mathbf{A})^2\psi - a^2\psi + b^2|\psi|^2\psi = 0 \tag{28}$$

We will also need Ampere's law (in the absence of electric fields)

$$\nabla \times B \;=\; \mu_0 \mathbf{J}. \tag{29}$$

We also need the plausible result that within Landau-Ginzberg theory, the current density is

$$J = \frac{1}{2i}\frac{q}{m}\left[\psi^*(\nabla - iq\mathbf{A})\psi - \psi(\nabla + iq\mathbf{A})\psi^*\right] \tag{30}$$

4.1. In Eq. (28), lets consider the situation where the first term is small compared to the second two. This is the "Thomas-Fermi" limit. Thus to lowest order $|\psi|^2 = (a/b)^2$ or more precisely

$$\psi = \frac{a}{b}e^{i\chi(\mathbf{r})}. \tag{31}$$

That is the amplitude of ψ is fixed, but its phase can vary in space.

Substitute this expression into Eq. (30) to find the current density as a function of χ and $\mathbf{A}$.

Solution 4.1 (3 points)**.**

$$\begin{aligned}\vec{J} &= \frac{1}{2i}\frac{q}{m}[\psi^*(\nabla - iq\vec{A})\psi - \psi(\nabla + iq\vec{A})\psi^*] \\ &= \frac{1}{2i}\frac{q}{m}\left[\frac{a}{b}e^{-i\chi(\vec{r})}\left(i\nabla(\chi(\vec{r})) - iq\vec{A}\right)\frac{a}{b}e^{i\chi(\vec{r})} - \frac{a}{b}e^{i\chi(\vec{r})}\left(-i\nabla(\chi(\vec{r})) + iq\vec{A}\right)\frac{a}{b}e^{-i\chi(\vec{r})}\right] \\ &= \frac{q}{m}\frac{a^2}{b^2}\left(\nabla(\chi(\vec{r})) - q\vec{A}\right)\end{aligned} \tag{32}$$

4.2. Take the curl of your expression for the current, and note that $\nabla \times (\nabla\chi) = 0$ to get an expression for the curl of the current which just depends on the magnetic field. [The coefficients a and b do not depend on space, so any derivatives of them should vanish.]

Solution 4.2 (2 points)**.** Using the fact that $\nabla \times \nabla(\chi(\vec{r})) = 0$,

$$\nabla \times \vec{J} = 0 - \frac{q}{m}\frac{a^2}{b^2}\nabla \times (q\vec{A}) = -\frac{q^2}{m}\frac{a^2}{b^2}\vec{B} \tag{33}$$

4.3. Take the curl of Eq. (29) to get London's equation,

$$\nabla \times (\nabla \times \mathbf{B}) = -\frac{1}{\lambda^2}\mathbf{B}. \tag{34}$$

What is the lengthscale λ?

Solution 4.3 (2 points)**.**

$$\nabla \times (\nabla \times \vec{B}) = \mu_0 \nabla \times \vec{J} = -\mu_0\frac{q^2}{m}\frac{a^2}{b^2}\vec{B} \tag{35}$$

We hence identify $\lambda = \frac{b}{aq}\sqrt{\frac{m}{\mu_0}}$.

4.4. Show that

$$\mathbf{B} = B_0 \hat{z} e^{-x/\lambda}, \tag{36}$$

is a solution to Eq. (34). Hence the magnetic field decays exponentially from the edge of the superconductor. The lengthscale λ is known as the "magnetic penetration depth" or the "London penetration depth."

Solution 4.4 (2 points)**.**

$$\nabla \times \left(\nabla \times \begin{pmatrix} 0 \\ 0 \\ B_0 e^{-x/\lambda} \end{pmatrix} \right) = \nabla \times \begin{pmatrix} 0 \\ \frac{B_0}{\lambda} e^{-x/\lambda} \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -\frac{B_0}{\lambda^2} e^{-x/\lambda} \end{pmatrix} \tag{37}$$

Hence we indeed have a solution to the London equation.

While nobody really thinks about it in the following way, we can now make the connection to the Higgs mechanism. We found a solution to Maxwell's equations (coupled to the matter field) with $\omega = 0$ and $k = i/\lambda$. It can be associated with a dispersion $\omega^2 = M^2 + k^2$. We see that $\lambda = 1/M$.

Problem 5. Feedback

5.1. How long did this homework take?

5.2. 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