PHY 6646 Spring 2002 – Homework 10

Due by 5 p.m. on Wednesday, May 1. No credit will be available for solutions submitted after this deadline.

Answer all questions. To gain full credit you should explain your reasoning and show all working. Please write neatly and include your name on the front page of your answers.

1. The *tight-binding model* is a simple model of electrons in ionic solids, where each electron spends most of its time localized in an ionic orbital, occasionally tunneling into an orbital on a nearby ion.

   A one-dimensional version of the tight-binding model is described by the second-quantized Hamiltonian

   $$H = -t \sum_{j=1}^{N} \sum_{\sigma} \left(c_{j,\sigma}^{\dagger} c_{j+1,\sigma} + c_{j+1,\sigma}^{\dagger} c_{j,\sigma} \right),$$

   where $c_{j,\sigma}$ annihilates an electron of spin $\sigma = \uparrow$ or $\downarrow$ in an orbital localized around site j, which is located at position $x_j = ja$. The lattice is subject to periodic boundary conditions, so $c_{j,\sigma} \equiv c_{j \pm N,\sigma}$. The set of creation and annihilation operators satisfies the standard fermionic anticommutation relations, i.e.,

   $$\{c_{j,\sigma}, c_{j',\sigma'}\} = \{c_{j,\sigma}^{\dagger}, c_{j',\sigma'}^{\dagger}\} = 0, \qquad \{c_{j,\sigma}, c_{j',\sigma'}^{\dagger}\} = \delta_{j,j'} \delta_{\sigma,\sigma'} I.$$

   Now consider a transformation to operators

   $$c_{k,\sigma} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{-ikx_j} c_{j,\sigma}.$$

   (a) Show that the $c_{k,\sigma}$'s also obey the standard fermionic anticommutation relations.

   (b) Write down the inverse transformation, i.e., $c_{j,\sigma}$ in terms of the $c_{k,\sigma}$'s, and hence deduce the allowed values of the wavevector k.

   (c) Show that the tight-binding Hamiltonian can be rewritten in the diagonal form

   $$H = \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^{\dagger} c_{k,\sigma}.$$

   Provide an explicit expression for the *dispersion*, ϵ_k.

   (d) Write down the ground states (plural) for three electrons, representing each state as a product of creation or annihilation operators acting on the vacuum state $|0\rangle$.

   The tight-binding model is simple to solve because it is bilinear in creation and annihilation operators. By contrast, the *Hubbard model*,

   $$H = -t \sum_{j=1}^{N} \sum_{\sigma} \left(c_{j,\sigma}^{\dagger} c_{j+1,\sigma} + c_{j+1,\sigma}^{\dagger} c_{j,\sigma} \right) + U \sum_{j=1}^{N} c_{j,\uparrow}^{\dagger} c_{j,\uparrow} c_{j,\downarrow}^{\dagger} c_{j,\downarrow},$$

   which includes Coulomb repulsion between spin-up and spin-down electrons on the same site, is extremely difficult to solve.

2. The Schrödinger equation can be written

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V - i\hbar\partial/\partial t\right)\psi = 0.$$

The potential V is assumed to be real. Multiplying this equation by ψ^* and then taking the imaginary part, one obtains a result that can be rewritten in the form of the continuity equation

$$\frac{\partial\rho}{\partial t} + \boldsymbol{\nabla}\cdot\mathbf{j} = 0,$$

where $\rho = \psi^*\psi$ is the probability and $\mathbf{j} = -(i\hbar/2m)(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*)$ is the probability current density.

   (a) By following the procedure described above, show that the Klein-Gordon equation can also be rewritten as a continuity equation, and determine the forms of ρ and $\mathbf{j}$ in this case.

   (b) Repeat part (a), but this time for the Dirac equation.

3. Shankar Exercise 20.2.2.