HW #10

1. Schrödinger field in momentum space

We start with the Lagrangian (sorry that ψ^* was missing in the second term in the problem set)

$L = \int d\vec{x}\left[\psi^* \, i\hbar\dot{\psi} - \psi^* \, \frac{-\hbar^2\nabla^2}{2m}\,\psi\right].$

We subsitute

$\psi = \sum_{\vec{p}} a(\vec{p})\,\frac{1}{L^{3/2}}\,e^{i\vec{p}\cdot\vec{x}/\hbar}.$

The first term is

$\int d\vec{x}\,\psi^*\,i\hbar\dot{\psi} = \int d\vec{x}\sum_{\vec{p}} a^*(\vec{p})\,\frac{1}{L^{3/2}}\,e^{-i\vec{p}\cdot\vec{x}/\hbar}\,i\hbar\sum_{\vec{q}}\dot{a}(\vec{q})\,\frac{1}{L^{3/2}}\,e^{i\vec{q}\cdot\vec{x}/\hbar}$

$= \sum_{\vec{p}}\sum_{\vec{q}} a^*(\vec{p})\,i\hbar\,\dot{a}(\vec{q})\,\frac{1}{L^3}\int d\vec{x}\,e^{-i\vec{p}\cdot\vec{x}/\hbar}\,e^{i\vec{q}\cdot\vec{x}/\hbar}$

$= \sum_{\vec{p}}\sum_{\vec{q}} a^*(\vec{p})\,i\hbar\,\dot{a}(\vec{q})\,\delta_{\vec{p},\vec{q}}$

$= \sum_{\vec{p}} a^*(\vec{p})\,i\hbar\,\dot{a}(\vec{p})$

The second term is

$\int d\vec{x}\left[-\psi^*\,\frac{-\hbar^2\nabla^2}{2m}\,\psi\right]$

$= \int d\vec{x}\left[-\sum_{\vec{p}} a^*(\vec{p})\,\frac{1}{L^{3/2}}\,e^{-i\vec{p}\cdot\vec{x}/\hbar}\,\frac{-\hbar^2\nabla^2}{2m}\sum_{\vec{q}} a(\vec{q})\,\frac{1}{L^{3/2}}\,e^{i\vec{q}\cdot\vec{x}/\hbar}\right]$

$= \int d\vec{x}\left[-\sum_{\vec{p}} a^*(\vec{p})\,\frac{1}{L^{3/2}}\,e^{-i\vec{p}\cdot\vec{x}/\hbar}\sum_{\vec{q}}\frac{\vec{q}^{\,2}}{2m}\,a(\vec{q})\,\frac{1}{L^{3/2}}\,e^{i\vec{q}\cdot\vec{x}/\hbar}\right]$

$= -\sum_{\vec{p}}\sum_{\vec{q}}\frac{\vec{q}^{\,2}}{2m}\,a^*(\vec{p})\,a(\vec{q})\,\frac{1}{L^3}\int d\vec{x}\,\frac{1}{L^{3/2}}\,e^{-i\vec{p}\cdot\vec{x}/\hbar}\,\frac{1}{L^{3/2}}\,e^{i\vec{q}\cdot\vec{x}/\hbar}$

$= -\sum_{\vec{p}}\sum_{\vec{q}}\frac{\vec{q}^{\,2}}{2m}\,a^*(\vec{p})\,a(\vec{q})\,\delta_{\vec{p},\vec{q}}$

$= -\sum_{\vec{p}}\frac{\vec{p}^{\,2}}{2m}\,a^*(\vec{p})\,a(\vec{p})$

Therefore, the Lagrangian is

$L = \sum_{\vec{p}}\left(a^*(\vec{p})\,i\hbar\,\dot{a}(\vec{p}) - \frac{\vec{p}^{\,2}}{2m}\,a^*(\vec{p})\,a(\vec{p})\right)$

It leads to the canonical commutation relation

$\left[a(\vec{p}),\,a^\dagger(\vec{q})\right] = \delta_{\vec{p},\vec{q}}$

and the Hamiltonian

$H = \sum_{\vec{p}}\frac{\vec{p}^{\,2}}{2m}\,a^*(\vec{p})\,a(\vec{p})$

Therefore $a^\dagger(\vec{p})$ creates a particle of momentum $\vec{p}$ and energy $\frac{\vec{p}^{\,2}}{2m}$.

2. Discretized Version

(a)

The canonical coordinate is c_i, and its conjugate momentum $\partial L \big/ \partial \dot{c}_i = i\hbar\, c_i^\dagger$, and hence $[c_i, i\hbar\, c_j^\dagger] = i\hbar\, \delta_{ij}$, or $[c_i, c_j^\dagger] = \delta_{ij}$.

The Hamiltonian is
$H = \sum_i i\hbar\, c_i^\dagger\, \dot{c}_i - L = \sum_{<i,j>} t(c_j^\dagger\, c_i + c_i^\dagger\, c_j)$.

(b)

In one-dimensional space, the sum over the nearest neighbor can be written down explicitly as
$H = \sum_{<i,j>} t(c_j^\dagger\, c_i + c_i^\dagger\, c_j) = t \sum_i (c_{i+1}^\dagger\, c_i + c_i^\dagger\, c_{i+1})$
Now we act the Hamiltonian on the state given in the problem,

$$
\begin{aligned}
H \sum_k c_k^\dagger\, e^{i k \kappa} \,|\, 0\rangle &= t \sum_i (c_{i+1}^\dagger\, c_i + c_i^\dagger\, c_{i+1}) \sum_k c_k^\dagger\, e^{i k \kappa} \,|\, 0\rangle \\
&= t \sum_i \sum_k (c_{i+1}^\dagger\, c_i\, c_k^\dagger + c_i^\dagger\, c_{i+1}\, c_k^\dagger)\, e^{i k \kappa} \,|\, 0\rangle \\
&= t \sum_i \sum_k (c_{i+1}^\dagger\, \delta_{ik} + c_i^\dagger\, \delta_{i+1,k})\, e^{i k \kappa} \,|\, 0\rangle \\
&= t \sum_k (c_{k+1}^\dagger + c_{k-1}^\dagger)\, e^{i k \kappa} \,|\, 0\rangle \\
&= t(\sum_k c_{k+1}^\dagger\, e^{i k \kappa} \,|\, 0\rangle + \sum_k c_{k-1}^\dagger\, e^{i k \kappa} \,|\, 0\rangle) \\
&= t(\sum_k c_k^\dagger\, e^{i (k-1) \kappa} \,|\, 0\rangle + \sum_k c_k^\dagger\, e^{i (k+1) \kappa} \,|\, 0\rangle) \\
&= 2\, t \cos\kappa \sum_k c_k^\dagger\, e^{i k \kappa} \,|\, 0\rangle
\end{aligned}
$$

Therefore, we see that it is indeed an eigenstate of the Hamiltonian with an eigenvalue $E = 2\, t \cos\kappa$.

To make the connection to the continuum theory, we need to regard the parameter κ as the momentum $\kappa = p\, a / \hbar$ where a is the lattice constant, and $t = -\hbar^2 / 2\, m\, a^2$ so that the eigenvalue is expanded in the small a limit as $E = \frac{-\hbar^2}{2\, m\, a^2} + \frac{p^2}{2\, m}$. This way, it has the form of the usual kinetic energy apart from the constant term.

Recall the Bloch wave discussed in 221A; the periodic potential always allows for "plane-wave-like" states because of the discrete translational invariance of the system. The tight-binding approximation is an extreme version of a periodic potential where the positions are restricted to the lattice sites by a steep potential.

(c)

In the limit of the small lattice spacings $a \to 0$, we regard the position of the sites continuous and can expand
$c_{i+1} = c_i + a \nabla c_i + \frac{a^2}{2} \nabla^2 c_i + O(a^3)$

The first term can be recast to the continuum form as
$\sum_i i \hbar c_i^* \dot{c}_i = \sum_i a \; i \hbar \left(\frac{c_i}{\sqrt{a}}\right)^* \frac{\dot{c}_i}{\sqrt{a}} \to \int d x \psi^* i \hbar \dot{\psi}$
with the identification $d x = a$, $\psi(x) = c_i / \sqrt{a}$. Note that the commutation relation makes sense as
$[\psi(x), \psi^\dagger(y)] = \left[\frac{c_i}{\sqrt{a}}, \frac{c_j{}^\dagger}{\sqrt{a}}\right] = \frac{\delta_{ij}}{a}$, which vanishes when $x \neq y$ while diverges when $x = y$ for $a \to 0$ as the detal function should.

The second term is expanded in power series in a,
$-t \sum_i (c_{i+1}{}^* c_i + c_i{}^* c_{i+1})$
$= -t \sum_i \left(\left(c_i + a \nabla c_i + \frac{a^2}{2} \nabla^2 c_i\right)^* c_i + c_i{}^* \left(c_i + a \nabla c_i + \frac{a^2}{2} \nabla^2 c_i\right)\right)$
$= -t \sum_i \left(c_i{}^* c_i + a \nabla c_i{}^* c_i + \frac{a^2}{2} \nabla^2 c_i{}^* c_i + c_i{}^* c_i + a c_i{}^* \nabla c_i + \frac{a^2}{2} c_i{}^* \nabla^2 c_i\right)$
$= -t \sum_i \left(2 c_i{}^* c_i + a (\nabla c_i{}^* c_i + c_i{}^* \nabla c_i) + \frac{a^2}{2} \left(\nabla^2 c_i{}^* c_i + \frac{a^2}{2} c_i{}^* \nabla^2 c_i\right)\right)$
Using the identifications found above, it becomes
$-t \int \frac{d x}{a} \left(2 \sqrt{a} \psi^* \sqrt{a} \psi + a \left(\nabla \sqrt{a} \psi^* \sqrt{a} \psi + \sqrt{a} \psi^* \nabla \sqrt{a} \psi\right) + \frac{a^2}{2} \left(\nabla^2 \sqrt{a} \psi^* \sqrt{a} \psi + \sqrt{a} \psi^* \nabla^2 \sqrt{a} \psi\right)\right)$
$= -t \int d x \left(2 \psi^* \psi + a (\nabla \psi^* \psi + \psi^\dagger \nabla \psi) + \frac{a^2}{2} (\nabla^2 \psi^* \psi + \psi^* \nabla^2 \psi)\right)$
The second term is a total derivative $(\nabla \psi^* \psi + \psi^* \nabla \psi) = \nabla(\psi^* \psi)$, and we ignore the surface terms. In the same way, the last term can be integrated by parts so that the derivatives act only on ψ but not on ψ^*. Finally using the identification $t = -\hbar^2 / 2 m a^2$ found in the previous problem,
$= \frac{\hbar^2}{2 m} \int d x (\frac{2}{a^2} \psi^* \psi + \psi^* \nabla^2 \psi)$.
The second term has precisely the form of the Lagrangian of the continuum Schrödinger field. The first term is proportional to the number operator $\int d x \psi^* \psi$. For a system with a fixed number of particles N, it gives rise to an additive constant to the Hamitonian $\frac{\hbar^2}{2 m a^2} N$. Even though it is formally divergent as $a \to 0$, a constant in the Hamiltonian does not have a physical meaning (except when the system is coupled to gravity) and we can safely drop it.

Of course, setting an infinite to zero makes everybody uncomfortable. If you don't like this, the discrete version of the Hamiltonian could have been written as
$-t \sum_{<i,j>} (c_i{}^* - c_j{}^*) (c_i - c_j)$
which avoids such a problem. I nonetheless used this form because you see it often in the literature (albeit with the opposite sign of t so that it is positive).