Quantum Traffic Wave Modeling

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1 Tight Binding Model for a 1D Ring

Let us consider non-interacting bosons on a strictly 1D ring of radius R and L sites. The single particle Hamiltonian is

$$H = \sum_{i=1}^{L} \epsilon_0 n_i - t \sum_{i=1}^{L} \left(a_{i+1}^\dagger a_i + a_i^\dagger a_{i+1} \right) \tag{1}$$

We define the ring by having periodicity: site $L+1$ being equivalent to site 1. We use the ansatz for bloch waves:

$$|\psi_{n\pm1}\rangle = e^{\pm ika}|\psi_n\rangle \tag{2}$$

We get the same dispersion relation as for the 1D tight binding model for a chain. Where a is the lattice spacing, which equals to $2\pi R/L$.

$$\epsilon(k) = \epsilon_0 - 2t\cos(ka) \tag{3}$$

For a finite ring, k takes discrete values. We can consider the additional phase of going around the whole ring to be 1.

$$e^{ikLa} = 1 \Longrightarrow k = \frac{2\pi}{aL}m \quad m \in \mathbb{Z} \tag{4}$$

For suitably small momenta, $k \ll \pi/a$, we can Taylor expand the energy. Setting $\epsilon_0 = 2t$ to yield the dispersion relation of a free particle with an effective mass determined by the properties of the lattice. Essentially, low momentum particles are unaware of the underlying lattice.

The energy spectrum has Z_2 symmetry about $k = 0$ with the ground state having zero k momentum, and thus zero m angular momentum. We want to break Z_2 symmetry about $k = 0$, and this can be done by passing magnetic flux through the ring.

2 Persistent Currents With Magnetic Flux

We now consider a continuum quantum ring with magnetic flux through the ring in such a way that the magnetic field is zero at the radius of the ring. By choosing circular cylindrical coordinate:

$$A_r = A_z = 0$$

$$A_\phi = \begin{cases} \frac{B_0 r}{2} & \text{if } r \leq r_c \\ \frac{B_0 r_c^2}{2r} = \frac{\Phi}{2\pi r} & \text{if } r > r_c \end{cases}$$

Such that there is flux $\Phi = \pi r_c^2 B_0$ through the ring. If the ring is in the field-free region, then the boson states only depend on the total flux penetrating the ring. Writing the potential term as, $V = e\phi - e\mathbf{A} \cdot \mathbf{v}$, we can write down the Lagrangian $L = T - V$ and then switch into the Hamiltonian formalism by finding the conjugate momentum. The general form of the Hamiltonian with an Electromagnetic potential energy term is

$$H = \frac{(\mathbf{p} - e\mathbf{A})^2}{2m} + e\phi_{EM} \tag{5}$$

For our case, we can immediately write down the TISE.

$$\frac{1}{2m}\left(-\frac{i\hbar}{R}\frac{\partial}{\partial\phi} - \frac{e\Phi}{2\pi R}\right)^2 \Psi(\phi) = \epsilon\Psi(\phi) \tag{6}$$

Due to the circle cylindrical symmetry, we use the ansatz $\psi_m = e^{im\phi}$. The dispersion relation written using angular momentum m is

$$\epsilon(m, \Phi) = \frac{\hbar^2}{2mR^2}\left(m - \frac{\Phi}{\Phi_0}\right)^2 \tag{7}$$

Where $\Phi_0 = h/e$ is the flux quantum. The result can be seen as a shift to the spectrum, such that the ground state has non-zero angular momentum.

One can think the same physical situation in a different manner. We can instead have a free-field Hamiltonian with twisted boundary conditions. *I.e. Ahranov-Bohm.* We first choose a gauge $\mathbf{A} = \nabla\chi$ such that $\mathbf{B} = \nabla \times \mathbf{A}$ is zero at the ring; in a strictly one-dimensional ring we can write $\chi(\phi) = \Phi\phi/(2\pi)$. We now write consider the following unitary transformations to the state and the Hamiltonian

$$\psi \to \psi' = U\psi \tag{8}$$

$$H \to H' = UHU^{-1} \tag{9}$$

By doing both transformations 8 and 9, the energy spectrum is preserved. We want the unitary transform to take the EM Hamiltonian H to the free-field Hamiltonian H'.

We define the unitary operator U as

$$U = e^{i\frac{e}{\hbar}\int \mathbf{A}d\mathbf{l}} = e^{-i\frac{e}{\hbar}\chi} \tag{10}$$

We act the unitary transform on the Hamiltonian in equation 6.

$$\Longrightarrow \frac{1}{2m}U\left(-\frac{i\hbar}{R}\partial_\phi - \frac{e\Phi}{2\pi R}\right)^2 U^{-1}\ f(\phi) \tag{11}$$

$$\Longrightarrow \frac{1}{2m}U\left(-\frac{i\hbar}{R}\partial_\phi - \frac{e\Phi}{2\pi R}\right)\left(U^{-1}\frac{-i\hbar}{R}\partial_\phi f(\phi)\right) \tag{12}$$

$$\Longrightarrow \frac{-\hbar^2}{2mR^2}\partial_\phi^2 f(\phi) \tag{13}$$

3 Tight Binding Model for a 1D Ring with Flux

We can write down the free-field Hamiltonian for this discrete model with flux by adding an Ahranov-Bohm phase term to the 1D Ring Hamiltonian in equation 1. The angle subtended by hopping from site i to site $i+1$ is $2\pi/L$

$$H = \sum_{i=1}^{L} \epsilon_0 n_i - t\sum_{i=1}^{L}\left(e^{-i2\pi\phi/L}a_{i+1}^\dagger a_i + e^{i2\pi\phi/L}a_i^\dagger a_{i+1}\right) \tag{14}$$

Where $\phi = \Phi/\Phi_0$. To find the dispersion relation, we can rewrite the Hamiltonian in terms of the basis states $a_1^\dagger|vac\rangle = |1\rangle$, $a_2^\dagger|vac\rangle = |2\rangle$ ...

$$H = \epsilon_0\sum_{n=1}^{L}|n\rangle\langle n| - t\sum_{n=1}^{L}\left(e^{-i2\pi\phi/L}|n+1\rangle\langle n| + e^{i2\pi\phi/L}|n\rangle\langle n+1|\right) \tag{15}$$

Considering a general state

$$|\Psi\rangle = \sum_m \psi_m|m\rangle \tag{16}$$

We can form the overlap $\langle p|H|\Psi\rangle = E\langle p|\Psi\rangle$

$$\epsilon_0\sum_n \psi_n\langle p|n\rangle - t\sum_n\left(\psi_n e^{-i2\pi\phi/L}\langle p|n+1\rangle + \psi_{n+1}e^{i2\pi\phi/L}\langle p|n\rangle\right) = E\sum_n\psi_n\langle p|n\rangle$$

$$\epsilon_0\psi_p - t\left(\psi_{p-1}e^{-i2\pi\phi/L} + \psi_{p+1}e^{i2\pi\phi/L}\right) = E\psi_p$$

Again, we use a Bloch wave ansatz $\psi_p = e^{ikpa}$ where $a = 2\pi R/L$ and k only taking discrete values shown in equation 4, resulting in

$$\epsilon_0 - t\left(e^{-i(ka+2\pi\phi/L)} + e^{i(ka+2\pi\phi/L)}\right) = E(k) \tag{17}$$

$$\epsilon_0 - 2t\cos(ka + 2\pi\phi/L) = E(k) \tag{18}$$

Assuming $ka + 2\pi\phi/L \ll \pi$, we Taylor expand the dispersion relation, and by choosing $\epsilon_0 = 2t$ the small argument expansion gives

$$E(k) \approx t\,(ka + 2\pi\phi/L)^2 \tag{19}$$

The new minimum of the dispersion relation does not occur at $k = 0$, but rather at $k = -2\pi\phi/(La)$

3.1 Probability current

Although the problem is stationary, *ie. the system is doing the same thing at all times, but there isn't time reversible symmetry due to the B field.*, we want to look at the probability current from each site.

We can consider the rate of change of occupation of site i by using Ehrenfest's Theorem. First we must define a positive circulation, we choose $i \to i+1$ to be a positive current. Units where $\hbar = c = 1$ are chosen and the Schrödinger picture is used.

$$\frac{d}{dt}\langle n_i\rangle = \frac{1}{i}\langle[n_i, H]\rangle \tag{20}$$

Only having nearest neighbor tunneling gives us the follow relation with the current $J_{i\to i+1}$

$$\frac{d}{dt}\langle n_i\rangle = J_{i-1\to i} - J_{i\to i+1} \tag{21}$$

Using the following commutation relations

$$[a_i, n_j] = a_i\delta_{ij}\ ,\ \left[a_i^\dagger, n_j\right] = -a_i^\dagger\delta_{ij}$$

We get [1]

$$\frac{d}{dt}\langle n_i\rangle = \frac{1}{i}\langle -te^{i2\pi\phi/L}c_i^\dagger c_{i+1} + te^{i2\pi\phi/L}c_{i+1}^\dagger c_i - te^{i2\pi\phi/L}c_i^\dagger c_{i-1} + te^{i2\pi\phi/L}c_{i-1}^\dagger c_i\rangle \tag{22}$$

By comparing with equation 21, we can write down the current $J_{i\to i+1}$

$$\begin{aligned} J_{i\to i+1} &= i\langle -te^{i2\pi\phi/L}c_i^\dagger c_{i+1} + te^{-i2\pi\phi/L}c_{i+1}^\dagger c_i\rangle \\ &= -2t\,\mathrm{Im}\left\{e^{-i2\pi\phi/L}\langle c_{i+1}^\dagger c_i\rangle\right\} \end{aligned} \tag{23}$$

[1] Full derivation of the probability current in the appendix

Considering a general state expressed in equation 16, we can find the expectation value

$$\begin{aligned} J_{i \to i+1} &\propto -2t\,\mathrm{Im}\big\{e^{-i2\pi\phi/L}e^{-ika}\big\} \\ &= 2t\sin(ka + 2\pi\phi/L) \end{aligned} \tag{24}$$

4 Initial Numerical Study

For the general many body case, we write down a Hubbard model corresponding to equation 14. The last term is the on-site Hubbard interaction term.

$$H = \sum_{i=1}^{L} \epsilon_0 n_i - t\sum_{i=1}^{L}\left(e^{-i2\pi\phi/L}a_{i+1}^{\dagger}a_i + e^{i2\pi\phi/L}a_i^{\dagger}a_{i+1}\right) + \frac{U}{2}\sum_{i=1}^{L} a_i^{\dagger}a_i^{\dagger}a_i a_i \tag{25}$$

We only want single occupation

$$\langle n_i \rangle = \{0, 1\} \tag{26}$$

To do this, we take the limit $U \to \infty$ and ignore the Hubbard interaction term in equation 25 and thus giving a Hardcore Boson model. What changes is the basis states. Our local Fock states with the max single occupancy restriction allows us to map our Hamiltonian to a spin system.

The matrix representation of the local basis at site i is

$$|0_i\rangle = (1, 0)^T \tag{27}$$

$$|1_i\rangle = (0, 1)^T \tag{28}$$

In this representation, the matrices the local creation and annihilation operators are

$$a = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \tag{29}$$

$$a^{\dagger} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \tag{30}$$

To get the whole Fock space, we take the tensor product of the local Fock spaces. We find the matrix representation of the basis states for the whole Foch space by taking every permutation of L Kronecker products of $(1, 0)^T$ and $(0, 1)^T$.

The matrix representation of the creation operator at site i is found by taking the appropriate number of Kronecker products with the identity matrix.

$$a_i^\dagger = \underbrace{\mathbb{1} \otimes \mathbb{1} \ldots \otimes \mathbb{1}}_{\text{i - 1 times}} \otimes a^\dagger \otimes \underbrace{\mathbb{1} \otimes \mathbb{1} \ldots \otimes \mathbb{1}}_{\text{L-i times}} \tag{31}$$

and likewise for the annihilation operator. The interpretation of equation 31 is that we apply the identity to all the other sites apart from site i, which we apply the local creation operator.

The single particle matrix elements of the creation and annihilation operators are all 0 because they do not conserve particle number.

$$\langle \Psi_{1,n} | a_j | \Psi_{1,m} \rangle = 0 \tag{32}$$

4.1 Numerical Dispersion Relation

The Hamiltonian matrix H can be thus be found by matrix multiplication and summing all the terms up in equation 25. The matrix size is $2^L \times 2^L$ and includes terms for single particle, two particles ... all the way up to L particles. Once

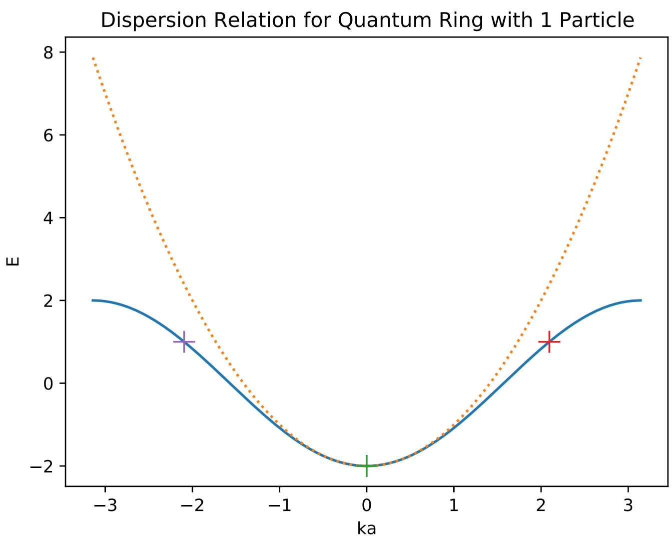

Figure 1: Plot of blue: exact dispersion relation for a single particle on a Quantum ring; orange: small momenta approximation for the dispersion relation. The three points are the eigenvalues for a single particle Hamiltonian for a Quantum ring with 3 sites. $\epsilon_0 = 0$, $a = 1$, $t = 1$, $\phi = 0$

the eigenvectors are found, we can find the k it corresponds to by finding the wavelength of the wavefunction.

$$\langle r|\Psi\rangle = \sum_m \psi_m \langle r|m\rangle \tag{33}$$

$$\Psi(r) = \sum_m \psi_m \xi_m(r) \tag{34}$$

I decided numerically that the sites are still labeled $1, 2, 3...$ even though python index starts at 0

4.2 Numerical Ground State Probability Current

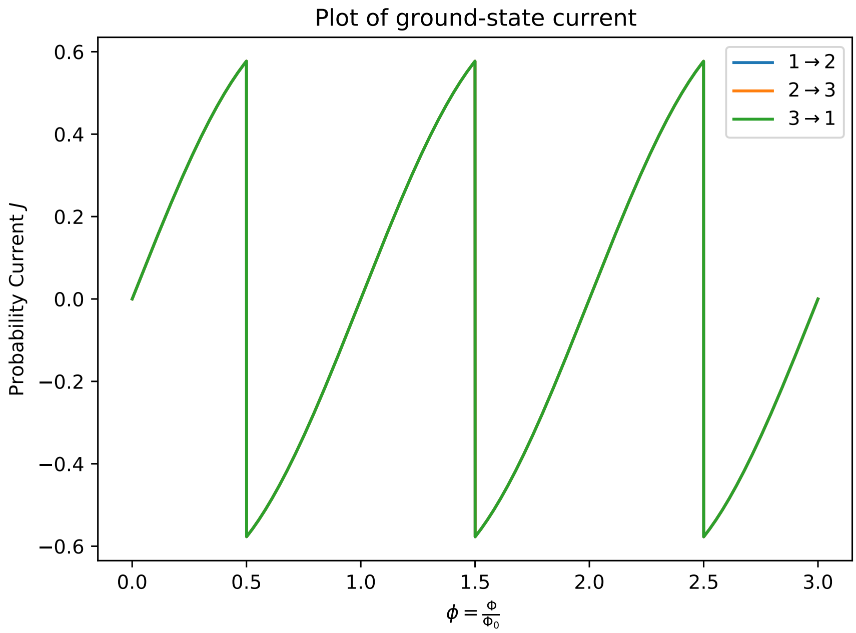

Figure 2: Plot of the probability current for the single particle ground state as a function of ϕ where $t = 1$. Note the current for different site hopping are all overlaid on each other, therefore all sites are equivalent. Another property of the relation to note is that it is periodic, with periodicity of 1. There is a maximum current at $0.5 - \epsilon$ (and its periodic repetitions) where $\epsilon > 0$ and is arbitrarily small, unlike for the classical car case where the cars there is no maximum speed for the cars.

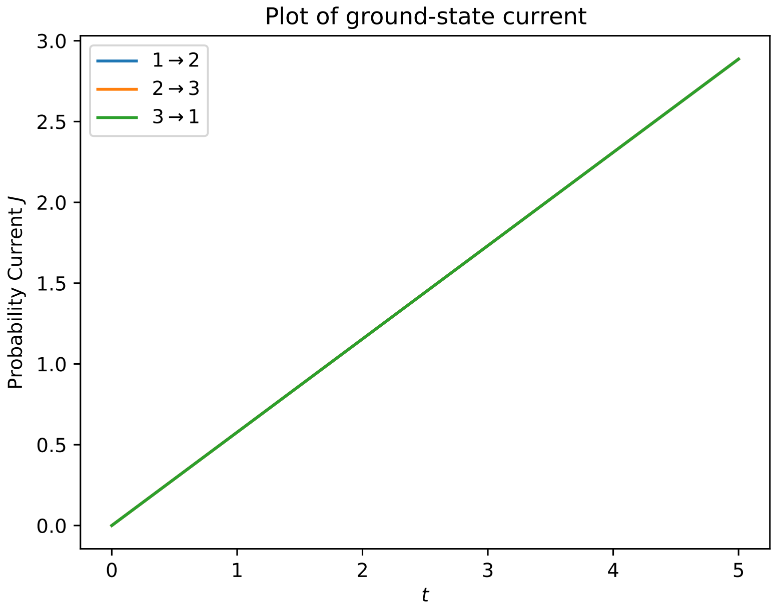

Figure 3: Plot of the probability current for the single particle ground state as a function of t where $\phi = 0.49999999$.The relation is linear, with gradient 0.577350 and intercept of 0