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1. Standard monolayer

We recall that

$$a_1 = a\begin{pmatrix}\frac{\sqrt{3}}{2}\\ \frac{1}{2}\end{pmatrix}, \qquad a_2 = a\begin{pmatrix}\frac{\sqrt{3}}{2}\\ -\frac{1}{2}\end{pmatrix} \qquad a_1^* = \frac{2\pi}{a}\begin{pmatrix}\frac{1}{\sqrt{3}}\\ 1\end{pmatrix}, \qquad a_2^* = \frac{2\pi}{a}\begin{pmatrix}\frac{1}{\sqrt{3}}\\ -1\end{pmatrix}$$

In reduced coordinates, with

$\mathcal{M} : \mathbb{T}^2 \simeq [0,1]^2 \to \Omega$,

$$\mathcal{M} := \frac{a}{2}\begin{pmatrix}\sqrt{3} & \sqrt{3}\\ 1 & -1\end{pmatrix} = \begin{pmatrix}a_1 & a_2\end{pmatrix}, \qquad \mathcal{M}^{-1} = \frac{1}{a}\begin{pmatrix}\frac{1}{\sqrt{3}} & 1\\ \frac{1}{\sqrt{3}} & -1\end{pmatrix}$$

and

$$2\pi\left(\mathcal{M}^{-1}\right)^* = \begin{pmatrix}a_1^* & a_2^*\end{pmatrix} = \frac{2\pi}{a}\begin{pmatrix}\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}}\\ 1 & -1\end{pmatrix} =: S$$

We know that $R_{\frac{2\pi}{3}}(ma^*) = \left(R^{\mathrm{red}}_{\frac{2\pi}{3}} m\right) a^*$ where

$$R^{\mathrm{red}}_{\frac{2\pi}{3}} = S^{-1} R_{\frac{2\pi}{3}} S = \mathcal{M}^* R_{\frac{2\pi}{3}} (\mathcal{M}^*)^{-1} = \begin{pmatrix}-1 & 1\\ -1 & 0\end{pmatrix}, \qquad R^{\mathrm{red}}_{-\frac{2\pi}{3}} = \begin{pmatrix}0 & -1\\ 1 & -1\end{pmatrix}$$

and

$$\mathcal{R}_{\frac{2\pi}{3}} f(x) = \sum_m f_m e^{i\left(R^{\mathrm{red}}_{\frac{2\pi}{3}} m\right) a^*\cdot x} = \sum_m f_{R^{\mathrm{red}}_{-\frac{2\pi}{3}} m} e^{ima^*\cdot x}$$

2. Rotated monolayer, by $\frac{\pi}{2}$

We define $J := \begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix} = R_{\frac{\pi}{2}}$, and then the rotated vectors are $\widetilde{a}_j = Ja_j$ so

$$\widetilde{a}_1 = a\begin{pmatrix}-\frac{1}{2}\\ \frac{\sqrt{3}}{2}\end{pmatrix}, \qquad \widetilde{a}_2 = a\begin{pmatrix}\frac{1}{2}\\ \frac{\sqrt{3}}{2}\end{pmatrix}, \qquad \widetilde{a}_1^* = \frac{2\pi}{a}\begin{pmatrix}-1\\ \frac{1}{\sqrt{3}}\end{pmatrix}, \qquad \widetilde{a}_2^* = \frac{2\pi}{a}\begin{pmatrix}1\\ \frac{1}{\sqrt{3}}\end{pmatrix}$$

so

$$\widetilde{\mathcal{M}} = \frac{a}{2}\begin{pmatrix}-1 & 1\\ \sqrt{3} & \sqrt{3}\end{pmatrix}, \qquad \widetilde{\mathcal{M}}^{-1} = \frac{1}{a}\begin{pmatrix}-1 & \frac{1}{\sqrt{3}}\\ 1 & \frac{1}{\sqrt{3}}\end{pmatrix}$$

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3. BM configuration

From [?], the BM Hamiltonian is

$$H = \begin{pmatrix} -i\sigma\nabla & T^c(x) \\ T^c(x)^* & -i\sigma\nabla \end{pmatrix},$$

where

$$\boxed{T_1 = \begin{pmatrix} w_0 & w_1 \\ w_1 & w_0 \end{pmatrix}, \quad T_2 = \begin{pmatrix} w_0 & w_1 e^{-i\phi} \\ w_1 e^{i\phi} & w_0 \end{pmatrix}, \quad T_3 = \begin{pmatrix} w_0 & w_1 e^{-i\overline{\phi}} \\ w_1 e^{i\overline{\phi}} & w_0 \end{pmatrix}}$$

and where, for $x \in \mathbb{R}^2$,

$$T^c(x) := \sum_{j=1}^{3} T_j e^{-iq_j^c \cdot x}, \qquad \widehat{T}_p = \sum_{j=1}^{3} T_j \delta_{p,q_j}$$

4. Rotation of $\frac{\pi}{2}$

From [?], we have vectors (in the reference, without the factor $\frac{4\pi}{a\sqrt{3}}$)

$$\widetilde{q}_1^c = \frac{4\pi}{a\sqrt{3}} \begin{pmatrix} 0 \\ -1 \end{pmatrix}, \qquad \widetilde{q}_{2,3}^c = \frac{4\pi}{a\sqrt{3}} \begin{pmatrix} \pm\frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix} = \frac{2\pi}{a} \begin{pmatrix} \pm 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix}$$

For them to be adapted to our lattice, we turn them and define $q_j^c := R_{-\frac{\pi}{2}} \widetilde{q}_j^c$, so that

$$q_2^c = a_2^*, \qquad q_3^c = a_1^*, \qquad q_1^c = \frac{4\pi}{a\sqrt{3}} \begin{pmatrix} -1 \\ 0 \end{pmatrix}$$

so after a rotation of $-\frac{\pi}{2}$, we have

$$T^c(x) = T_1 e^{-iq_1^c \cdot x} + T_2 e^{-ia_2^* \cdot x} + T_3 e^{-ia_1^* \cdot x}$$

On reduced coordinates, we have

$$T(x) = T^c(\mathcal{M}x) = \sum_{j=1}^{3} T_j e^{-ix \cdot \mathcal{M}^* q_j^c} = \sum_{j=1}^{3} T_j e^{i2\pi x \cdot q_j}$$

where $q_j := -\mathcal{M}^* q_j^c / 2\pi$, so

$$q_2 = \begin{pmatrix} 0 \\ -1 \end{pmatrix}, q_3 = \begin{pmatrix} -1 \\ 0 \end{pmatrix}, q_1 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Writing a drawing and placing the q_i's, we have

$$R_{\frac{2\pi}{3}} q_1 = q_2, \qquad R_{\frac{2\pi}{3}} q_2 = q_3, \qquad R_{\frac{2\pi}{3}} q_3 = q_1$$

so

$$\mathcal{R}_{\frac{2\pi}{3}} T(x) = T_1 e^{-iq_2 x} + T_2 e^{-iq_3 x} + T_3 e^{-iq_1 x}$$

We don't have $\mathcal{R}_{\frac{2\pi}{3}} T = T$ but this is true for the diagonal elements and for the off-diagonal, there exists X such that $\mathcal{R}_{\frac{2\pi}{3}} (\tau_X T) = \tau_X T$.

5. Without rotation

Without rotation, we have $q_j := -\widetilde{\mathcal{M}}^* \widetilde{q}_j^c / 2\pi$ so

$$T(x) = T^c(\widetilde{\mathcal{M}} x) = \sum_{j=1}^{3} T_j e^{-ix \cdot \widetilde{\mathcal{M}}^* \widetilde{q}_j^c} = \sum_{j=1}^{3} T_j e^{i 2\pi x \cdot \widetilde{q}_j}$$

$$\boxed{q_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad q_2 = \begin{pmatrix} 0 \\ -1 \end{pmatrix}, \qquad q_3 = \begin{pmatrix} -1 \\ 0 \end{pmatrix}}$$

Or

$$\boxed{T(x) = \sum_{j=1}^{3} T_j e^{i q_j a^* \cdot x}}$$

Since $T_j^* = T_j$, then $T(-x)^* = T(x)$

5.1. **Basis.**

We define $e_m := \frac{1}{\sqrt{|\Omega|}} e^{i m a^* \cdot x}$, and

$$e_{\alpha,m} := e_\alpha \otimes e_m = e_\alpha \frac{e^{i m a^* \cdot x}}{\sqrt{|\Omega|}}, \qquad \text{where } e_1 := \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \ldots$$

6. Operators in basis

For a general $W = \sum_k W^{ika^* \cdot x}$, we have

$$\begin{aligned}
M_{IJ} &:= \left\langle e_{\alpha,n}, \begin{pmatrix} 0 & W \\ W^* & 0 \end{pmatrix} e_{\beta,m} \right\rangle \\
&= \sum_k \left(\delta_{\alpha \in \{1,2\}}^{\beta \in \{3,4\}} \delta_{m+k-n} \left\langle e_{\alpha_1}, W_k e_{\beta_2} \right\rangle + \delta_{\alpha \in \{3,4\}}^{\beta \in \{1,2\}} \delta_{m-k-n} \left\langle e_{\alpha_2}, W_k^* e_{\beta_1} \right\rangle \right) \\
&= \delta_{\alpha \in \{1,2\}}^{\beta \in \{3,4\}} \left\langle e_{\alpha_1}, W_{n-m} e_{\beta_2} \right\rangle + \delta_{\alpha \in \{3,4\}}^{\beta \in \{1,2\}} \left\langle e_{\alpha_2}, W_{m-n}^* e_{\beta_1} \right\rangle \\
&= \delta_{\alpha \in \{1,2\}}^{\beta \in \{3,4\}} \left(W_{n-m} \right)_{\alpha_1 \beta_2} + \delta_{\alpha \in \{3,4\}}^{\beta \in \{1,2\}} \overline{\left(W_{m-n} \right)_{\beta_1 \alpha_2}}
\end{aligned}$$

and M is also Hermitian.

For a general $V = \sum_k V^{ika^* \cdot x}$, we have

$$\left\langle e_{\alpha,n}, \begin{pmatrix} V & 0 \\ 0 & V \end{pmatrix} e_{\beta,m} \right\rangle = \delta_{\alpha \in \{1,2\}}^{\beta \in \{1,2\}} \left(V_{n-m} \right)_{\alpha_1 \beta_1} + \delta_{\alpha \in \{3,4\}}^{\beta \in \{3,4\}} \left(V_{n-m} \right)_{\alpha_2 \beta_2}$$

For a general $A = \begin{pmatrix} A_1 \\ A_2 \end{pmatrix}$, $A_j = \sum_k \left(A_j \right)_k e^{ika^* \cdot x}$, we compute

$$\begin{aligned}
&\left\langle e_{\alpha,n}, \begin{pmatrix} 0 & A \cdot (-i\nabla) \\ A^* \cdot (-i\nabla) & 0 \end{pmatrix} e_{\beta,m} \right\rangle \\
&\quad = \delta_{\alpha \in \{1,2\}}^{\beta \in \{3,4\}} \left((ma^*)_1 \left((A_1)_{n-m} \right)_{\alpha_1 \beta_2} + (ma^*)_2 \left((A_2)_{n-m} \right)_{\alpha_1 \beta_2} \right) \\
&\qquad + \delta_{\alpha \in \{3,4\}}^{\beta \in \{1,2\}} \left((ma^*)_1 \overline{\left((A_1)_{m-n} \right)_{\beta_1 \alpha_2}} + (ma^*)_2 \overline{\left((A_2)_{m-n} \right)_{\beta_1 \alpha_2}} \right)
\end{aligned}$$

7. Symmetries

7.1. **Particle-hole.** we have

$$\mathcal{S}\begin{pmatrix}0 & \mathbb{V}\\ \mathbb{V}^* & 0\end{pmatrix}\mathcal{S} = -\begin{pmatrix}0 & \mathbb{V}^*(-x)\\ \mathbb{V}(-x) & 0\end{pmatrix} = -\begin{pmatrix}0 & \mathbb{V}\\ \mathbb{V}^* & 0\end{pmatrix}$$

we also have, for any operator A,

$$\mathcal{S}\begin{pmatrix}A & 0\\ 0 & A\end{pmatrix}\mathcal{S} = P\begin{pmatrix}A & 0\\ 0 & A\end{pmatrix}P$$

where $Pu(x) := u(-x)$. Hence

$$\mathcal{S}\begin{pmatrix}\sigma\cdot\nabla & 0\\ 0 & \sigma\cdot\nabla\end{pmatrix}\mathcal{S} = -\begin{pmatrix}\sigma\cdot\nabla & 0\\ 0 & \sigma\cdot\nabla\end{pmatrix}$$

but since $P\sigma\cdot kP = \sigma\cdot k$,

$$\mathcal{S}\begin{pmatrix}\sigma\cdot(-i\nabla+k) & 0\\ 0 & \sigma\cdot(-i\nabla+k)\end{pmatrix}\mathcal{S} = \begin{pmatrix}\sigma\cdot(-i\nabla-k) & 0\\ 0 & \sigma\cdot(-i\nabla-k)\end{pmatrix}$$

so it is not $\mathcal{S}$ symmetric ! We have $T(-x)^* = T(x)$ hence defining

$$\mathcal{S}u(x) := i\begin{pmatrix}0 & -\mathbb{1}_{2\times 2}\\ \mathbb{1}_{2\times 2} & 0\end{pmatrix}u(-x)$$

we should have that

$$\mathcal{S}H\mathcal{S} = -H$$

We compute

$$\begin{aligned}\mathcal{S}_{IJ} = \langle e_{\alpha,n}, \mathcal{S}e_{\beta,n}\rangle &= i\left\langle e_{\alpha,n}, \begin{pmatrix}-e_{\beta_2,-m}\\ e_{\beta_1,-m}\end{pmatrix}\right\rangle\\ &= i\delta_{m+n}\left(\delta^{\beta\in\{1,2\}}_{\alpha\in\{3,4\}}\delta_{\beta_1-\alpha_2} - \delta^{\beta\in\{3,4\}}_{\alpha\in\{1,2\}}\delta_{\beta_2-\alpha_1}\right)\end{aligned}$$

8. Numerics

We have

$$\begin{aligned}\sigma\cdot(-i\nabla+k) &= \sigma_1(-i\partial_1+k_1)+\sigma_2(-i\partial_2+k_2)\\ &= \begin{pmatrix}0 & -i(\partial_1-i\partial_2)+\overline{k_{\mathbb{C}}}\\ -i(\partial_1+i\partial_2)+k_{\mathbb{C}} & 0\end{pmatrix}\end{aligned}$$

where

$$\sigma_1 = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \qquad \sigma_2 = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$$

so, with $k_{\mathbb{C}} := k_1 + ik_2$,

$$\begin{aligned}\sigma\cdot(-i\nabla+k)\begin{pmatrix}1\\0\end{pmatrix}e_m &= (ma^*+k)_{\mathbb{C}}\begin{pmatrix}0\\1\end{pmatrix}e_m\\ \sigma\cdot(-i\nabla+k)\begin{pmatrix}0\\1\end{pmatrix}e_m &= \overline{(ma^*+k)_{\mathbb{C}}}\begin{pmatrix}1\\0\end{pmatrix}e_m\end{aligned}$$

Then

$$\begin{pmatrix} \sigma\cdot(-i\nabla+k) & 0 \\ 0 & \sigma\cdot(-i\nabla+k) \end{pmatrix} e_{1,m} = (ma^*+k)_{\mathbb{C}}\, e_{2,m}$$
$$\begin{pmatrix} \sigma\cdot(-i\nabla+k) & 0 \\ 0 & \sigma\cdot(-i\nabla+k) \end{pmatrix} e_{2,m} = \overline{(ma^*+k)_{\mathbb{C}}} e_{1,m}$$
$$\begin{pmatrix} \sigma\cdot(-i\nabla+k) & 0 \\ 0 & \sigma\cdot(-i\nabla+k) \end{pmatrix} e_{3,m} = (ma^*+k)_{\mathbb{C}}\, e_{4,m}$$
$$\begin{pmatrix} \sigma\cdot(-i\nabla+k) & 0 \\ 0 & \sigma\cdot(-i\nabla+k) \end{pmatrix} e_{4,m} = \overline{(ma^*+k)_{\mathbb{C}}} e_{3,m}$$

and for $V_{ij} := E_{ij}v_{ij}$ where v_{ij} is a potential in $\mathbb{R}^2$ and $E_{ij} := |e_i\rangle\langle e_j|$ being the 4×4 matrix having a one at line i and column j,

$$V_{\gamma,\eta}e_{\alpha,m} = \delta_{\eta,\alpha}e_\gamma \otimes v_{\gamma,\eta}e_m$$

and we recall that $ve_m = \sum_k v_k e_{k+m}$ hence

$$\langle e_n, ve_m\rangle = v_{n-m}$$

and

$$\langle e_{\beta,n}, V_{\gamma,\eta}e_{\alpha,m}\rangle = \delta_{\eta,\alpha}\delta_{\beta,\gamma}\langle e_n, v_{\gamma,\eta}e_m\rangle = \delta_{\eta,\alpha}\delta_{\beta,\gamma}\left(v_{\gamma,\eta}\right)_{n-m}$$

9. Eigenvalue equation

We have $H\psi = ES\psi$ is equivalent to $S^*H\psi = ES^*S\psi$ and

$$(S^*S)^{-\frac{1}{2}} S^*H (S^*S)^{-\frac{1}{2}} \psi = E\psi$$

and in the code we define $S_2 := (S^*S)^{-\frac{1}{2}} S^*$ and $S_1 = (S^*S)^{-\frac{1}{2}}$

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