Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Generation of large spin and valley currents in a quantum pump based on molybdenum disulfide

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SUPPORTING INFORMATION

Scattering Matrix Elements

In the matrix form, Eq.(1) can be written as

$$H = \begin{bmatrix} \frac{\Delta}{2} + V_i - hs & \hbar v_F(\tau k_x - ik_y) \\ \hbar v_F(\tau k_x + ik_y) & -\frac{\Delta}{2} + \lambda\tau s + V_i - hs \end{bmatrix} \tag{S.1}$$

The eigenvalue problem does have the following form

$$(H - EI)\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{bmatrix} \frac{\Delta}{2} + V_i - hs - E & \hbar v_F(\tau k_x - ik_y) \\ \hbar v_F(\tau k_x + ik_y) & -\frac{\Delta}{2} + \lambda\tau s + V_i - hs - E \end{bmatrix}\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = 0. \tag{S.2}$$

Using Eq. (S.2), we have

$$\psi_2 = q\psi_1 \tag{S.3}$$

where

$$q = -\frac{\Delta/2 + V_i - hs - E}{\hbar v_F(\tau k_x - ik_y)} \tag{S.4}$$

The normalization condition, $|\psi_1|^2 + |\psi_2|^2 = 1$, gives

$$\psi_1 = \frac{1}{\sqrt{(1+q^2)}}, \quad \psi_2 = q\psi_1$$

Eq. (S.2) for eigenvalues gives rise to

$$\left(\frac{\Delta}{2} + V_i - hs - E\right)\left(-\frac{\Delta}{2} + \lambda\tau s + V_i - hs - E\right) = (\hbar v_F k)^2 \tag{S.5}$$

where $k = \sqrt{k_x^2 + k_y^2}$. To distinguish the wave vectors in the scattering region from those for incoming/outgoing electrons, we use the superscript II for the wave vectors of the scattering region. Translational invariance along the y-direction requires that the transverse wave vector k_y be conserved throughout the system. For a given k_y we have $k_x = \sqrt{k^2 - k_y^2}$ for the x-component of the wave vector of incoming/outgoing waves and $k_x^{II} = \sqrt{(k^{II})^2 - k_y^2}$ for the x-component of the wave vector in the scattering region. Having wave vectors in all the regions, the wave functions for incoming waves, scattering region and outgoing waves are as follows

$$\begin{aligned} \psi^{in} &= \frac{e^{ik_y y}e^{ik_x x}}{\sqrt{1+|q(k_x)|^2}}\begin{pmatrix} 1 \\ q(k_x) \end{pmatrix} + r\frac{e^{ik_y y}e^{-ik_x x}}{\sqrt{1+|q(-k_x)|^2}}\begin{pmatrix} 1 \\ q(-k_x) \end{pmatrix}; \\ \psi^{II} &= a\frac{e^{ik_y y}e^{ik_x^{II} x}}{\sqrt{1+|q^{II}(k_x^{II})|^2}}\begin{pmatrix} 1 \\ q^{II}(k_x^{II}) \end{pmatrix} + b\frac{e^{ik_y y}e^{-ik_x^{II} x}}{\sqrt{1+|q^{II}(-k_x^{II})|^2}}\begin{pmatrix} 1 \\ q^{II}(-k_x^{II}) \end{pmatrix}; \\ \psi^{out} &= t\frac{e^{ik_y y}e^{ik_x x}}{\sqrt{1+|q(k_x)|^2}}\begin{pmatrix} 1 \\ q(k_x) \end{pmatrix}. \end{aligned} \tag{S.6}$$

in which $q(k_x) = -\frac{\Delta/2 - E}{\hbar v_F(\tau k_x - ik_y)}$ and $q^{II}(k_x^{II}) = -\frac{\Delta/2 + V_i - hs - E}{\hbar v_F(\tau k_x^{II} - ik_y)}$. The transport coefficients r and t are obtained by matching the wave functions at the two borders, x' and x'', of the scattering region:

$$\psi^{in}(x') = \psi^{II}(x') \tag{S.7}$$

$$\psi^{II}(x'') = \psi^{out}(x'') \tag{S.8}$$

After straithforward calculation we have:

$$r = \frac{A_9 q(k_x) - A_{11}}{A_{12} - A_{10} q(k_x)} \tag{S.9}$$

$$t = \frac{\sqrt{1 + |q(k_x)|^2}(A_{11}A_{10} - A_9 A_{12})}{e^{ik_x x''}(A_{10} q(k_x) - A_{12})} \tag{S.10}$$

in which

$$A_9 = A_5\frac{e^{ik_x^{II} x''}}{\sqrt{1 + |q^{II}(k_x^{II})|^2}} + A_7\frac{e^{-ik_x^{II} x''}}{\sqrt{1 + |q^{II}(-k_x^{II})|^2}}$$

$$A_{10} = A_6\frac{e^{ik_x^{II} x''}}{\sqrt{1 + |q^{II}(k_x^{II})|^2}} + A_8\frac{e^{-ik_x^{II} x''}}{\sqrt{1 + |q^{II}(-k_x^{II})|^2}}$$

$$A_{11} = A_5\frac{e^{ik_x^{II} x''} q^{II}(k_x^{II})}{\sqrt{1 + |q^{II}(k_x^{II})|^2}} + A_7\frac{e^{-ik_x^{II} x''} q^{II}(-k_x^{II})}{\sqrt{1 + |q^{II}(-k_x^{II})|^2}}$$

$$A_{12} = A_6\frac{e^{ik_x^{II} x''} q^{II}(k_x^{II})}{\sqrt{1 + |q^{II}(k_x^{II})|^2}} + A_8\frac{e^{-ik_x^{II} x''} q^{II}(-k_x^{II})}{\sqrt{1 + |q^{II}(-k_x^{II})|^2}}$$

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and

$$A_5 = \frac{e^{i(k_x - k_x^{II})x'}[q(k_x) - q^{II}(-k_x^{II})]}{q^{II}(k_x^{II}) - q^{II}(-k_x^{II})} \frac{\sqrt{1+|q^{II}(k_x^{II})|^2}}{\sqrt{1+|q(k_x)|^2}}$$

$$A_6 = \frac{e^{-i(k_x + k_x^{II})x'}[q(-k_x) - q^{II}(-k_x^{II})]}{q^{II}(k_x^{II}) - q^{II}(-k_x^{II})} \frac{\sqrt{1+|q^{II}(k_x^{II})|^2}}{\sqrt{1+|q(-k_x)|^2}}$$

$$A_7 = \frac{e^{i(k_x + k_x^{II})x'}[q(k_x) - q^{II}(k_x^{II})]}{q^{II}(-k_x^{II}) - q^{II}(k_x^{II})} \frac{\sqrt{1+|q^{II}(k_x^{II})|^2}}{\sqrt{1+|q(k_x)|^2}}$$

$$A_8 = \frac{e^{i(k_x^{II} - k_x)x'}[q(-k_x) - q^{II}(k_x^{II})]}{q^{II}(-k_x^{II}) - q^{II}(k_x^{II})} \frac{\sqrt{1+|q^{II}(k_x^{II})|^2}}{\sqrt{1+|q(-k_x)|^2}}$$

We note that r' and t' can be obtained simply by interchanging x' and x'', k_x and $-k_x$, k_x^{II} and $-k_x^{II}$. Therefore, the elements of scattering matrix for a region between x' and x'' are $S = [(r,t)^T(t',r')^T]$. The elements of scattering matrix for the whole system can be easily obtained from those of the individual regions with straightforward calculations.