Extramize the functional that describes defects in crystals

$$\mathcal{F}[\theta(x)] = \int_{-\infty}^{\infty} \left[\frac{\kappa}{2} \left(\frac{\mathrm{d}\theta}{\mathrm{d}x} \right)^2 + V(1 - \cos\theta(x)) \right] \mathrm{d}x \tag{1}$$

subject to boundary conditions $\theta(-\infty) = 0$, $\theta(\infty) = 2\pi$. Further, find the energy cost $E = \mathcal{F}[\Theta]$ for Θ that extramizes F.

We read off the functional

$$F(\theta, \theta') = \frac{\kappa}{2}\theta'^2 + V(1 - \cos\theta). \tag{2}$$

To use Euler-Lagrange equation, we first prepare

$$\frac{\partial F}{\partial \theta} = v \sin \theta; \quad \frac{\partial F}{\partial \theta'} = \kappa \theta'. \tag{3}$$

Then E-L gives

$$\frac{\mathrm{d}}{\mathrm{d}x}(\kappa\theta') - V\sin\theta = 0$$

$$\Rightarrow \theta'' = \frac{1}{\xi^2}\sin\theta, \quad \xi = \sqrt{\frac{\kappa}{V}}.$$
(4)

This non-linear ODE can be solved indirectly had we noticed that F is independent of x, and so Beltrami identity applies:

$$F - \theta' \frac{\mathrm{d}F}{\mathrm{d}\theta'} = C$$

$$\Rightarrow \frac{\kappa}{2} \theta'^2 - V(1 - \cos \theta) = C$$
(5)

Boundary conditions give $x \to \pm \infty \Rightarrow \theta' = 0, \cos \theta = 1 \Longrightarrow C = 0$. Thus we solve

$$\frac{\kappa}{2}\theta'^2 = V(1 - \cos\theta) \Rightarrow \theta'^2 = \frac{4}{\xi^2}\sin^2\left(\frac{\theta}{2}\right) \tag{6}$$

to get

$$\frac{\mathrm{d}\theta}{2\sin\left(\frac{\theta}{2}\right)} = \frac{\mathrm{d}x}{\xi}$$

$$\Rightarrow \frac{1}{2}\csc\left(\frac{\theta}{2}\right)\mathrm{d}\theta = \frac{1}{\xi}\mathrm{d}x.$$
(7)

Since $\int \csc u \, du = \ln(\tan(\frac{u}{2}))$, we take integration on both sides over an arbidrary range $[x_0, x]$, this yields

$$\theta = \arctan\left[\frac{\exp(x - x_0)}{\xi}\right] \equiv \Theta.$$
 (8)

The corresponding functional is thus (with $\frac{\kappa}{2}\Theta'^2=V(1-\cos\Theta)$)

$$F(\Theta,\Theta') = 4V \sin^2 \left(\frac{\theta}{2}\right) = 4V \operatorname{sech}^2 \left(\frac{x-x_0}{\xi}\right). \tag{9}$$

The energy cost is therefore

$$E = \int_{-\infty}^{\infty} F \, \mathrm{d}x = 4V \int_{-\infty}^{\infty} \mathrm{sech}^2 \left(\frac{x - x_0}{\xi} \right) \mathrm{d}x = 8V \xi = \boxed{8\sqrt{\kappa V}}.$$
 (10)

Apply calculus of variations to find coupled equations for ψ and \boldsymbol{A} that extramize \mathcal{F} , where \mathcal{F} is the free energy functional of a superconductor:

$$\mathcal{F}[\psi(\mathbf{r}), \mathbf{A}(\mathbf{r})] = \int_{V} \left(-|\psi|^{2} + \frac{1}{2} |\psi|^{4} + \left| \left(-\frac{i}{\kappa} \nabla - \mathbf{A} \right) \psi \right|^{2} + \mathbf{H}^{2} \right) dV$$
(11)

Let $D_i = -\frac{i}{\kappa}\partial_i - A_i, H_i = \varepsilon_{ijk}\partial_j A_k,$ and define

$$F(\psi, \psi^*, \mathbf{A}, \partial_i \psi, \partial_i \psi^*, \partial_i A_j) = -|\psi|^2 + \frac{1}{2} |\psi|^4 + |D_i \psi|^2 + H_i^2.$$
(12)

Here we use a genralized Euler Lagrange equation for $F(\varphi_i, \partial_i \varphi_i)$:

$$\frac{\partial F}{\partial \varphi_j} - \partial_i \left(\frac{\partial F}{\partial (\partial_i \varphi_j)} \right) = 0. \tag{13}$$

We will deal with $\varphi_j=\psi^*$ and $\varphi_j=A_j$ separately. For $\varphi_j=\psi^*,$ we have

$$\begin{split} \frac{\partial F}{\partial \psi^*} &= -\psi + |\psi|^2 \psi - A_i D_i \psi, \\ \frac{\partial F}{\partial (\partial_i \psi^*)} &= \frac{\partial}{\partial (\partial_i \psi^*)} \left(-\frac{i}{\kappa} \partial_i \psi - A_i \psi \right) \left(\frac{i}{\kappa} \partial_i \psi^* - A_i \psi^* \right) = \frac{i}{\kappa} D_i \psi. \end{split} \tag{14}$$

Then EL reads

$$\frac{\partial F}{\partial \psi^*} - \partial_i \left(\frac{\partial F}{\partial (\partial_i \psi^*)} \right) = 0$$

$$\Rightarrow -\psi + |\psi|^2 \psi - A_i D_i \psi - \frac{i}{\kappa} \partial_i D_i \psi = 0$$

$$\Rightarrow \boxed{-\psi + |\psi|^2 \psi + D_i D_i \psi = 0.}$$
(15)

On the other hand, for $\varphi_j=A_j,$ defining $D_i^\dagger=\left(\frac{i}{\kappa}\partial_i-A_i\right)$ we have

$$\begin{split} \frac{\partial F}{\partial A_{j}} &= -\left[\psi D_{j}^{\dagger} \psi^{*} + \psi^{*} D_{j} \psi\right], \\ \frac{\partial F}{\partial \left(\partial_{i} A_{j}\right)} &= 2H_{k} \frac{\partial H_{k}}{\partial \left(\partial_{i} A_{j}\right)} = 2H_{k} \varepsilon_{kij} \\ \Rightarrow \partial_{i} \left(\frac{\partial F}{\partial \left(\partial_{i} A_{j}\right)}\right) &= 2\varepsilon_{kij} \partial_{i} H_{k} = -2(\nabla \times \mathbf{H})_{j}. \end{split} \tag{16}$$

The EL equation thus reads

$$\begin{split} - \left[\psi D_j^{\dagger} \psi^* + \psi^* D_j \psi \right] + 2 (\nabla \times \boldsymbol{H})_j &= 0 \Longrightarrow \boxed{\nabla \times \boldsymbol{H} = \boldsymbol{J},} \\ \text{where } J_i &= \frac{1}{2} \left[\psi D_i^{\dagger} \psi^* + \psi^* D_i \psi \right] = \frac{1}{2} \left[\frac{i}{\kappa} (\psi \partial_i \psi^* - \psi^* \partial_i \psi) - (\psi A_i \psi^* + \psi^* A_i \psi) \right. \end{aligned} \\ &= \frac{1}{2} \left[\frac{i}{\kappa} (-2i \operatorname{Im}(\psi^* \partial_i \psi)) - 2A_i |\psi|^2 \right] = \frac{1}{\kappa} \operatorname{Im}(\psi^* \partial_i \psi) - A_i |\psi|^2. \end{split}$$

Collecting above, we arrive at

$$\begin{cases} -\psi + |\psi|^2 \psi + D_i D_i \psi = 0 \\ \nabla \times \boldsymbol{H} = \boldsymbol{J} \\ \boldsymbol{J} = \frac{1}{\kappa} \operatorname{Im}(\psi^* \nabla \psi) - \boldsymbol{A} |\psi|^2 \end{cases} . \tag{18}$$

Find the kink configuration $\varphi(x)$ and its energy cost for the functional

$$\mathcal{F}[\varphi] = \int_{-\infty}^{\infty} \left[\frac{\kappa}{2} \left(\frac{\mathrm{d}\varphi}{\mathrm{d}x} \right)^2 + \frac{V}{4} (\varphi^2 - \varphi_0^2)^2 \right] \mathrm{d}x \tag{19}$$

subject to boundary conditions $\varphi(-\infty) = -\varphi_0, \varphi(\infty) = \varphi_0$.

We read off the functional

$$F(\varphi,\varphi') = \frac{\kappa}{2}\varphi'^2 + \frac{V}{4}(\varphi^2 - \varphi_0^2)^2. \tag{20}$$

Similar to P1, we notice that F is independent of x, and so Beltrami identity applies:

$$F - \varphi' \frac{\mathrm{d}F}{\mathrm{d}\varphi'} = C$$

$$\Rightarrow -\frac{\kappa}{2}\varphi'^2 + \frac{V}{4}(\varphi^2 - \varphi_0^2)^2 = C$$
(21)

Boundary conditions give $x\to\pm\infty\Rightarrow \varphi'=0, \varphi^2=\varphi_0^2\Longrightarrow C=0.$ Thus we solve

$$\frac{\kappa}{2}\varphi'^2 = \frac{V}{4}(\varphi^2 - \varphi_0^2)^2 \Rightarrow \varphi' = \sqrt{\frac{V}{2\kappa}}(\varphi_0^2 - \varphi^2) \tag{22}$$

to get

$$\frac{\mathrm{d}\varphi}{\varphi_0^2 - \varphi^2} = \sqrt{\frac{V}{2\kappa}} \,\mathrm{d}x. \tag{23}$$

Since $\int \frac{\mathrm{d}u}{a^2-u^2} = \frac{1}{a} \operatorname{artanh}\left(\frac{u}{a}\right)$, we take integration on both sides over an arbitrary range $[x_0,x]$. this yields

$$\frac{1}{\varphi_0} \operatorname{artanh}\left(\frac{\varphi}{\varphi_0}\right) = \sqrt{\frac{V}{2\kappa}}(x - x_0). \tag{24}$$

Defining a characteristic length $\xi = \sqrt{\frac{\kappa}{V\varphi_0^2}}$, the equation simplifies to $\operatorname{artanh}\left(\frac{\varphi}{\varphi_0}\right) = \frac{x-x_0}{\sqrt{2}\xi}$.

$$\varphi = \varphi_0 \tanh \left[\frac{x - x_0}{\sqrt{2}\xi} \right] \equiv \Phi.$$
 (25)

The corresponding functional is thus (with $\frac{\kappa}{2}\Phi'^2 = \frac{V}{4}(\Phi^2 - \varphi_0^2)^2)F(\Phi,\Phi') = \kappa\Phi'^2 = \frac{\kappa\varphi_0^2}{2\xi^2}\operatorname{sech}^4\left(\frac{x-x_0}{\sqrt{2}\xi}\right) = \frac{V}{2}\varphi_0^4\operatorname{sech}^4\left(\frac{x-x_0}{\sqrt{2}\xi}\right)$. The energy cost is therefore $E = \int_{-\infty}^{\infty}F\operatorname{d}x = \frac{V}{2}\varphi_0^4\int_{-\infty}^{\infty}\operatorname{sech}^4\left(\frac{x-x_0}{\sqrt{2}\xi}\right)\operatorname{d}x$ Using the standard integral

$$\int_{-\infty}^{\infty} \operatorname{sech}^{4}(u) \, \mathrm{d}u = \frac{4}{3},\tag{26}$$

we get

$$E = \frac{2\sqrt{2}}{3}\varphi_0^3\sqrt{\kappa V}.$$
 (27)

Consider a functional of three functions

$$G[y_1, y_2, y_3] = \int_{x_0}^{x_1} F[x, y, y'] \, \mathrm{d}x, \quad F[x, y, y'] = \frac{1}{2} \sum_{i,j=1}^{3} g_{ij}(y) y_{i'} y_{j'} - U(y), \tag{28}$$

where g_{ij} is a symmetric matrix that depends on y. Derive the system's of Euler-Lagrange equations that extramize G. Use Chistoffel symbols to simplify your result.

Using Einstein summation convention, and denote $\partial_k u = \frac{\partial u}{\partial u_k}$, we write

$$F = \frac{1}{2}g_{ij}y_{i'}y_{j'} - U(y). \tag{29}$$

And the Euler-Lagrange equation elements are found as follows

$$\frac{\partial F}{\partial y_k} = \frac{\partial}{\partial y_k} \left[\frac{1}{2} g_{ij} y_{i'} y_{j'} - U(y) \right] = \frac{1}{2} (\partial_k g_{ij}) y_{i'} y_{j'} - \partial_k U,$$

$$\frac{\partial F}{\partial y_k'} = \frac{1}{2} g_{ij} \partial_k (y_{i'} y_{j'}) = \frac{1}{2} g_{ij} (\delta_{ik} y_{j'} + y_{i'} \delta_{jk}) = g_{kj} y_{j'}$$
(30)

$$\frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{\partial F}{\partial y_k'} \right) = \frac{\mathrm{d}}{\mathrm{d}x} (g_{kj} y_{j'}) = \frac{\mathrm{d}g_{kj}}{\mathrm{d}x} y_j' + \frac{\mathrm{d}}{\mathrm{d}x} y_j' g_{kj}
= \frac{\mathrm{d}y_l}{\mathrm{d}x} \frac{\partial}{\partial y_l} g_{kj} y_j' + y_j'' g_{kj} = (\partial_l g_{kj}) y_l' y_j' + g_{kj} y_j''.$$
(31)

E-L equation reads

$$\frac{1}{2} (\partial_k g_{ij}) y_i' y_j' - \partial_k U - (\partial_l g_{kj}) y_i' y_j' - g_{kj} y_j'' = 0$$
(32)

Rearranging

$$g_{kj}y_j'' + \partial_l g_{kj}y_l'y_j' - \frac{1}{2}\partial_k g_{ij}y_i'y_j' + \partial_k U = 0.$$

$$(33)$$

We can use the identity $g_{mk}g_{kj}=\delta(mj)$ to simplify:

$$y_m'' + g_{mk} \underbrace{\left[\partial_l g_{kj} - \frac{1}{2} \partial_k g_{ij}\right] y_l' y_j'}_{(*)} + g_{mk} \partial_k U = 0.$$

$$\tag{34}$$

Since $y'_l y'_j$ is symmetric in l, j, we can symmetrize the term

$$\partial_l g_{kj} y_l' y' j = \frac{1}{2} \left[\partial_l g_{kj} + \partial_j g_{kl} \right] y_l' y_j'. \tag{35}$$

Then (*) becomes

$$\frac{1}{2} \left[\partial_l g_{kj} + \partial_j g_{kl} - \partial_k g_{ij} \right] y_l' y_j' = \Gamma_{lj}^k y_l' y_j', \tag{36}$$

and we arrive at a simplified form:

$$y_m'' + g_{mk} \Gamma_{lj}^k y_l' y_j' + g_{mk} \partial_k U = 0.$$

$$(37)$$

Consider the Lagrangian density for a one-dimensional electron-phonon system:

$$\mathcal{L} = \frac{i}{2} \left(\dot{\psi} \psi^* - \psi \dot{\psi}^* \right) - \frac{1}{2} |\partial_x \psi|^2 + \frac{1}{2} (\partial_t u)^2 - \frac{s^2}{2} (\partial_x u)^2 + g(\partial_x u) |\psi|^2. \tag{38}$$

First, derive the equations of motion for the complex field $\psi(x,t)$ and the real field u(x,t). Then, find a traveling-wave solution (polaron) of the form $\psi(x,t)=e^{i(ax-bt)}\varphi(x-Vt)$ and u(x,t)=U(x-Vt). Finally, calculate the total energy E(V) of this solution and find the ground state energy E_0 .

1. Equations of Motion from Variational Principle

The Lagrangian density is given by $\mathcal{L} = \mathcal{L}_{\psi} + \mathcal{L}_{u} + \mathcal{L}_{\psi u}$:

$$\mathcal{L} = \frac{i}{2} \left(\dot{\psi} \psi^* - \psi \dot{\psi}^* \right) - \frac{1}{2} |\partial_x \psi|^2 + \frac{1}{2} (\partial_t u)^2 - \frac{s^2}{2} (\partial_x u)^2 + g(\partial_x u) |\psi|^2 \tag{39}$$

The equations of motion are derived from the Euler-Lagrange equations.

Equation for $\psi(x,t)$

We vary with respect to the independent field ψ^* . The Euler-Lagrange equation is:

$$\frac{\partial \mathcal{L}}{\partial \psi^*} - \partial_t \left(\frac{\partial \mathcal{L}}{\partial \dot{\psi}^*} \right) - \partial_x \left(\frac{\partial \mathcal{L}}{\partial (\partial_x \psi^*)} \right) = 0 \tag{40}$$

The required partial derivatives are:

$$\frac{\partial \mathcal{L}}{\partial \psi^*} = \frac{i}{2} \dot{\psi} + g(\partial_x u) \psi \tag{41}$$

$$\frac{\partial \mathcal{L}}{\partial \dot{\psi}^*} = -\frac{i}{2}\psi \tag{42}$$

$$\frac{\partial \mathcal{L}}{\partial (\partial_x \psi^*)} = -\frac{1}{2} (\partial_x \psi) \tag{43}$$

Substituting these into the equation gives:

$$\left(\frac{i}{2}\dot{\psi} + g(\partial_x u)\psi\right) - \partial_t \left(-\frac{i}{2}\psi\right) - \partial_x \left(-\frac{1}{2}\partial_x \psi\right) = 0 \tag{44}$$

$$\Rightarrow \frac{i}{2}\dot{\psi} + g(\partial_x u)\psi + \frac{i}{2}\dot{\psi} + \frac{1}{2}\partial_x^2\psi = 0 \tag{45}$$

This simplifies to the first equation of motion:

$$i\partial_t \psi = -\frac{1}{2} \partial_x^2 \psi - g(\partial_x u) \psi \eqno(46)$$

Equation for u(x,t)

We vary with respect to the real field u:

$$\frac{\partial \mathcal{L}}{\partial u} - \partial_t \left(\frac{\partial \mathcal{L}}{\partial (\partial_t u)} \right) - \partial_x \left(\frac{\partial \mathcal{L}}{\partial (\partial_x u)} \right) = 0 \tag{47}$$

The partial derivatives are:

$$\frac{\partial \mathcal{L}}{\partial u} = 0 \tag{48}$$

$$\frac{\partial \mathcal{L}}{\partial (\partial_t u)} = \partial_t u \tag{49}$$

$$\frac{\partial \mathcal{L}}{\partial (\partial_x u)} = -s^2 (\partial_x u) + g|\psi|^2 \tag{50}$$

Substituting these yields:

$$0 - \partial_t(\partial_t u) - \partial_x(-s^2 \partial_x u + g|\psi|^2) = 0 \tag{51}$$

This simplifies to the second equation of motion:

$$\partial_t^2 u - s^2 \partial_x^2 u + g \partial_x (|\psi|^2) = 0$$
(52)

2. Traveling-Wave Solution

We seek a solution where the electron and the string deformation propagate together at a velocity V. We introduce the co-moving coordinate $\xi = x - Vt$ and use the ansatz:

$$\psi(x,t) = e^{i(ax-bt)}\varphi(\xi), \quad u(x,t) = U(\xi)$$
(53)

where $\varphi(\xi)$ is a real-valued profile function, and a,b are constants. The derivatives transform as $\partial_t = -V \frac{\mathrm{d}}{\mathrm{d}\xi}$ and $\partial_x = \frac{\mathrm{d}}{\mathrm{d}\xi}$.

Applying these transformations to the ansatz (denoting $\frac{d}{d\xi}$ with a prime):

$$\partial_{\iota}\psi = e^{i(ax - bt)}(-ib\varphi - V\varphi') \tag{54}$$

$$\partial_x \psi = e^{i(ax - bt)} (ia\varphi + \varphi') \tag{55}$$

$$\partial_x^2 \psi = e^{i(ax-bt)} (-a^2 \varphi + 2ia\varphi' + \varphi'') \tag{56}$$

$$\partial_t u = -VU', \quad \partial_t^2 u = V^2 U'' \tag{57}$$

$$\partial_x u = U', \quad \partial_x^2 u = U'' \tag{58}$$

Substituting these into the first equation of motion and canceling the phase factor $e^{i(ax-bt)}$ gives:

$$i(-ib\varphi - V\varphi') = -\frac{1}{2}(-a^2\varphi + 2ia\varphi' + \varphi'') - gU'\varphi$$

$$\tag{59}$$

$$\Rightarrow b\varphi - iV\varphi' = \frac{a^2}{2}\varphi - ia\varphi' - \frac{1}{2}\varphi'' - gU'\varphi \tag{60}$$

Separating the real and imaginary parts:

· Imaginary Part:

$$-V\varphi' = -a\varphi' \Longrightarrow a = V. \tag{61}$$

This aligns the phase velocity with the group velocity, a feature of Galilean invariance.

Real Part:

$$b\varphi = \frac{V^2}{2}\varphi - \frac{1}{2}\varphi'' - gU'\varphi. \tag{62}$$

Rearranging gives:

$$-\frac{1}{2}\varphi'' - gU'\varphi = \left(b - \frac{V^2}{2}\right)\varphi \tag{63}$$

Define $\mu := b - \frac{V^2}{2}$, which represents the energy of the electron in the co-moving frame. The equation becomes:

$$-\frac{1}{2}\varphi''(\xi) - gU'(\xi)\varphi(\xi) = \mu\varphi(\xi) \tag{64}$$

Next, substituting the ansatz into the second equation of motion gives:

$$V^{2}U'' - s^{2}U'' + g\frac{\mathrm{d}}{\mathrm{d}\xi}(\varphi^{2}) = 0 \Longrightarrow (V^{2} - s^{2})U'' + g(\varphi^{2})' = 0$$
 (65)

Solving the Coupled ODEs

We integrate Equation 65 with respect to ξ . For a localized polaron, we assume the fields vanish at infinity $(\varphi(\xi) \to 0$ and $U'(\xi) \to 0$ as $|\xi| \to \infty$), which sets the integration constant to zero:

$$(V^2 - s^2)U' + g\varphi^2 = 0 \Longrightarrow U'(\xi) = \frac{g}{s^2 - V^2}\varphi^2(\xi)$$

$$\tag{66}$$

For a localized "bright soliton" solution to exist, the induced self-interaction for the electron must be attractive. Substituting U' into Equation 63:

$$-\frac{1}{2}\varphi'' - \frac{g^2}{s^2 - V^2}\varphi^3 = \mu\varphi \tag{67}$$

The nonlinear term $-\frac{g^2}{s^2-V^2}\varphi^3$ is attractive if the coefficient is negative, which requires $s^2-V^2>0$, or |V|< s. The polaron must travel slower than the speed of sound in the medium. We also need $\mu<0$ for a bound state. Let $\mu=-\nu$ where $\nu>0$. The equation is:

$$\varphi'' = 2\nu\varphi - \frac{2g^2}{s^2 - V^2}\varphi^3 \tag{68}$$

This is a standard nonlinear Schrödinger (NLS) equation. The solution is of the form:

$$\varphi(\xi) = A \operatorname{sech}(\alpha \xi) \tag{69}$$

Substituting this form back into the NLS equation gives the relations: $\alpha^2 = 2\nu$ and $A^2 = \frac{2\nu(s^2 - V^2)}{g^2} = \frac{\alpha^2(s^2 - V^2)}{g^2}$.

We impose the normalization condition for a single electron, $\int_{-\infty}^{\infty} |\psi|^2 dx = \int_{-\infty}^{\infty} \varphi^2 d\xi = 1$:

$$\int_{-\infty}^{\infty} A^2 \operatorname{sech}^2(\alpha \xi) \, \mathrm{d}\xi = A^2 \left[\frac{1}{\alpha} \tanh(\alpha \xi) \right]_{-\infty}^{\infty} = \frac{2A^2}{\alpha} = 1 \tag{70}$$

Using $A^2=rac{lpha^2(s^2-V^2)}{g^2}$, we get $rac{2}{lpha}rac{lpha^2(s^2-V^2)}{g^2}=1$, which solves for lpha:

$$\alpha = \frac{g^2}{2(s^2 - V^2)} \tag{71}$$

From this, we find the other parameters:

$$A^{2} = \frac{\alpha}{2} = \frac{g^{2}}{4(s^{2} - V^{2})}, \quad \nu = \frac{\alpha^{2}}{2} = \frac{g^{4}}{8(s^{2} - V^{2})^{2}}$$
 (72)

3. System Energy E(V)

The Hamiltonian (energy) density is derived from the Lagrangian density: $\mathcal{H} = \sum \pi_i \dot{\varphi}_i - \mathcal{L}$.

$$\pi_{\psi} = \frac{\partial \mathcal{L}}{\partial \dot{\psi}} = \frac{i}{2} \psi^*, \quad \pi_u = \frac{\partial \mathcal{L}}{\partial \dot{u}} = \partial_t u$$
 (73)

$$\mathcal{H} = \left(\frac{i}{2}\psi^*\right)\dot{\psi} + \left(-\frac{i}{2}\psi\right)\dot{\psi}^* + (\partial_t u)(\partial_t u) - \mathcal{L}$$

$$= \frac{1}{2}|\partial_x \psi|^2 + \frac{1}{2}(\partial_t u)^2 + \frac{s^2}{2}(\partial_x u)^2 - g(\partial_x u)|\psi|^2)$$
(74)

The total energy is $E(V) = \int_{-\infty}^{\infty} \mathcal{H} \, \mathrm{d}x$. We substitute the traveling wave solution into the terms of \mathcal{H} :

$$\left|\partial_x \psi\right|^2 = \left|e^{i(Vx - bt)}(\varphi' + iV\varphi)\right|^2 = (\varphi')^2 + V^2 \varphi^2 \tag{75}$$

•
$$(\partial_t u)^2 = (-VU')^2 = V^2(U')^2$$
 (76)

• Using $U' = \frac{g}{s^2 - V^2} \varphi^2$, the terms involving u become:

$$\frac{1}{2} (V^2 + s^2) (U')^2 - gU'\varphi^2 = \frac{1}{2} (V^2 + s^2) \frac{g^2}{(s^2 - V^2)^2} \varphi^4 - \frac{g^2}{s^2 - V^2} \varphi^4 = -\frac{g^2(s^2 - 3V^2)}{2(s^2 - V^2)^2} \varphi^4$$
 (78)

The total energy integral is:

$$E(V) = \int_{-\infty}^{\infty} \left[\frac{1}{2} \left((\varphi')^2 + V^2 \varphi^2 \right) - \frac{g^2 (s^2 - 3V^2)}{2(s^2 - V^2)^2} \varphi^4 \right] d\xi$$
 (79)

We evaluate the separate integrals using our solution for φ :

$$\int \frac{1}{2} V^2 \varphi^2 \, d\xi = \frac{1}{2} V^2 \quad \int \varphi^2 \, d\xi = \frac{1}{2} V^2$$
 (80)

(from normalization).

$$\int \frac{1}{2} (\varphi')^2 d\xi = \int \frac{1}{2} A^2 \alpha^2 \operatorname{sech}^2(\alpha \xi) \tanh^2(\alpha \xi) d\xi = \frac{A^2 \alpha}{3} = \frac{\left(\frac{\alpha}{2}\right) \alpha}{3} = \frac{\alpha^2}{6} = \frac{\nu}{3} = \frac{g^4}{24(s^2 - V^2)^2}$$
(81)

.

$$\int \varphi^4 \, \mathrm{d}\xi = \int A^4 \, \mathrm{sech}^4(\alpha \xi) \, \mathrm{d}\xi = A^4 \frac{4}{3\alpha} = \left(\frac{\alpha}{2}\right)^2 \frac{4}{3\alpha} = \frac{\alpha}{3} = \frac{g^2}{6(s^2 - V^2)} \tag{82}$$

.

Combining these results:

$$E(V) = \frac{1}{2}V^2 + \frac{g^4}{24(s^2 - V^2)^2} - \frac{g^2(s^2 - 3V^2)}{2(s^2 - V^2)^2} \left(\frac{g^2}{6(s^2 - V^2)}\right)$$

$$= \frac{1}{2}V^2 + \frac{g^4}{24(s^2 - V^2)^3} [(s^2 - V^2) - 2(s^2 - 3V^2)]$$

$$= \frac{1}{2}V^2 + \frac{g^4}{24(s^2 - V^2)^3} (5V^2 - s^2)$$
(83)

This gives the final energy as a function of velocity for the subsonic polaron, valid for |V| < s:

$$E(V) = \frac{V^2}{2} + \frac{g^4(5V^2 - s^2)}{24(s^2 - V^2)^3}$$
(84)

Ground State Energy E_0

The ground state energy is the energy of a static polaron, found by setting V = 0.

$$E_0 = E(0) = \frac{0}{2} + \frac{g^4(0 - s^2)}{24(s^2 - 0)^3} = \boxed{\frac{-g^4}{24s^4}}$$
(85)

The negative energy confirms that the formation of a static polaron is energetically favorable, representing a stable bound state.