$E(\vec{x}) = f(x_0, \ldots, x_N)$

Problema para el estado base.

$\to \underset{\{x_n\}}{\text{Min}}\ E(\vec{x})$?

$\hookrightarrow$ Serie de equaciones

$$\vec{f}(\vec{x}) = 0$$

Antes $\to$ Ecs. del Cruce BCS-BEC.
(Leggett).

$\boxed{\text{Bose Hubbard}}$ en aproximación de campo medio (MFT)

$\hookrightarrow$ Base de Fock.
Para la QPT

SF – MI.

Bose Hubbard.

$$\hat{\mathcal{H}} = -t \sum_{\langle ij \rangle}' (\hat{b}_i^{+} \hat{b}_j + H.c.)$$

$$+ \frac{U}{2} \sum_i' \hat{n}_i(\hat{n}_i - 1) - \mu \sum_i \hat{n}_i$$

Multiplicador de Lagrange.

Si uno quiere
$\rho = cte$.

Entonces hay que encontrar el $\mu \rightarrow \rho(t, U, \mu)$

$\rho = \langle \hat{n}_i \rangle$ con condiciones periódicas, sistema homogeneo

(Weak Coupling (Acoplamiento Débil)

$$\hat{b}_j = \frac{1}{\sqrt{M}} \sum_k \hat{a}_k e^{i\vec{k}\cdot\vec{r}_j}$$

$$\hat{b}_j^{+} = \frac{1}{\sqrt{M}} \sum_k \hat{a}_k^{+} e^{-i\vec{k}\cdot\vec{r}_j}$$

$M = \#$ sitios.

Momentum space

$$\varepsilon(\vec{k}) = 2J \sum_{m=1}^{d} \cos(k_m a)$$

En Fourier

E. Cin. + Pot. Quím.

$$\hat{\mathcal{H}} = \sum_{\vec{k}} \underbrace{[-\varepsilon(\vec{k}) - \mu] \hat{a}_k^{+} \hat{a}_k}_{\text{Diagonal}}$$

$$+ \frac{U}{2M} \sum_{\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4} \delta_{\vec{k}_1+\vec{k}_2, \vec{k}_3+\vec{k}_4} *$$

$* \; a^{+}_{k_1} a^{+}_{k_2} a_{k_3} a_{k_4}$.

$$\frac{U}{J} \to 0 \quad \therefore \quad |\Phi\rangle \approx (a_0^{+})^N |0\rangle$$

Método de Bogoliubov.

$\langle \hat{a}_0 \rangle = \langle \hat{a}_0^{+} \rangle \approx \sqrt{N_0}$ el BEC

$\hat{a}_0 = \sqrt{N_0} + \delta \hat{a}_0 \leftarrow$ fluctuaciones arriba del BEC.

Despues ....

$$\hat{\mathcal{H}} = \underbrace{N_0 \left(-zt - \mu + \frac{U}{2} n_0\right) + \sqrt{N_0}\,(U n_0 - tz - \mu)(\hat{a}_0 + \hat{a}_0^{+})}_{\text{BEC.}}$$

$$+ \sum_{\vec{k}}{}' (-\varepsilon(\vec{k}) - \mu) \hat{a}_{\vec{k}} \hat{a}_{\vec{k}}$$

$$+\frac{U n_0}{2}\sum_{\vec{k}}\left(4\hat{a}_k^{+}\hat{a}_k+\hat{a}_k\hat{a}_{-k}+\hat{a}_k^{+}\hat{a}_{-k}^{+}\right)$$

$n_0=\frac{N_0}{M}$ fracción de condensado

$z=2d$ número de coordinación

Transformación canónica de operadores.

$$\left.\begin{aligned}\hat{c}_{\vec{k}}&=u_{\vec{k}}\hat{a}_{\vec{k}}+v_{\vec{k}}\hat{a}_{-\vec{k}}^{+}\\ \hat{c}_{-\vec{k}}^{+}&=v_{\vec{k}}^{*}\hat{a}_{\vec{k}}+u_{\vec{k}}^{*}\hat{a}_{-\vec{k}}^{+}\end{aligned}\right\}$$ Conservan Relaciones de Conmutación

$$\tilde{\mathcal{H}}=-\frac{U n_0 N_0}{2}+\frac{1}{2}\sum_{\vec{k}}\left(\hbar\omega_{\vec{k}}+\epsilon(\vec{k})-zt\right.$$

$- U n_0)$

$$+ \sum_{\vec{k}} \hbar\omega_{\vec{k}} \hat{C}^{+}_{\vec{k}} \hat{C}_{\vec{k}}$$

$$\hbar\omega_{\vec{k}} = \sqrt{(zJ - \epsilon(\vec{k}))^2 + 2Un_0(zJ - \epsilon(\vec{k}))}$$

para $\vec{k} \to 0$

$$\hbar\omega_{\vec{k}} \approx |\vec{k}| a \sqrt{J} \sqrt{J|k|^2 a^2 + 2Un_0}$$

No ha $- = MI$

y SI -

porque no hay gap.

para $\forall U$.

Teoría Efectiva que describa

$\to SI - MI$

el escenario físico. $\rightarrow$ Si MI

Desacoplamiento:

$$\rightarrow (b_i^+ - \langle b_i^+ \rangle)(b_j - \langle b_j \rangle) \approx 0$$

$$b_i^+ b_j \approx + \langle b_i^+ \rangle b_j + \langle b_j \rangle b_i^+ - \langle b_i^+ \rangle \langle b_j \rangle$$

$$\psi_i = \langle b_i \rangle \ , \ \psi_i^* = \langle b_i^+ \rangle$$

$$\psi_i = \psi_i^* \longrightarrow \psi_i \in \mathbb{R} \ , \ \psi_i = \psi_j = \psi$$

$$b_i^+ b_j \approx \psi (b_j + b_i^+) - \psi^2$$

$$E.Cin \rightarrow -t \sum_{\langle ij \rangle} (b_i^+ b_j + H.c.)$$

$$\simeq -zt(\psi(b+b^+) - \psi^2)M$$

E. In + Pot Quim.

$$\rightarrow \simeq \frac{U}{2} M(\hat{n}^2 - \hat{n}) - \mu M \hat{n}.$$

$$\rightarrow \tilde{E} = \frac{E}{M} = \overbrace{-zt(\psi(\hat{b}+\hat{b}^{+}) - \psi^2)}^{\text{E. Cin.}} + \frac{U}{2}(\hat{n}^2) - \left(\mu + \frac{U}{2}\right)\hat{n}$$

$$\hat{b}|n\rangle = \sqrt{n}\,|n-1\rangle$$

$$\hat{b}^{+}|n\rangle = \sqrt{n+1}\,|n\rangle$$

$$\hat{n}|n\rangle = n|n\rangle$$

Todo el Hamiltoniano es ahora tridiagonal

$$\psi \neq 0 \rightarrow SF$$

$$\psi = 0 \rightarrow MI. \rightarrow |1\rangle$$

$$\boxed{\text{Teoría de perturbaciones} \quad U \gg t}$$

$$\tilde{\mathcal{H}} = -\psi(\hat{b}^\dagger + \hat{b}) + \psi^2 - \tilde{\mu}\hat{n} + \tilde{U}\hat{n}(\hat{n}-1)$$

$$\tilde{\mu} = \frac{\mu}{zt}, \quad \tilde{U} = \frac{U}{zt}$$

$$\tilde{\mathcal{H}} = \underline{\underline{\tilde{U}\tilde{\mathcal{H}}_0}} + \underbrace{\psi V}_{\text{pert.}} + \psi^2 \quad \text{cte.}$$

$$\boxed{\tilde{\mathcal{H}}_0 = -\frac{\tilde{\mu}}{\tilde{U}}\hat{n} + \hat{n}(\hat{n}-1)}$$

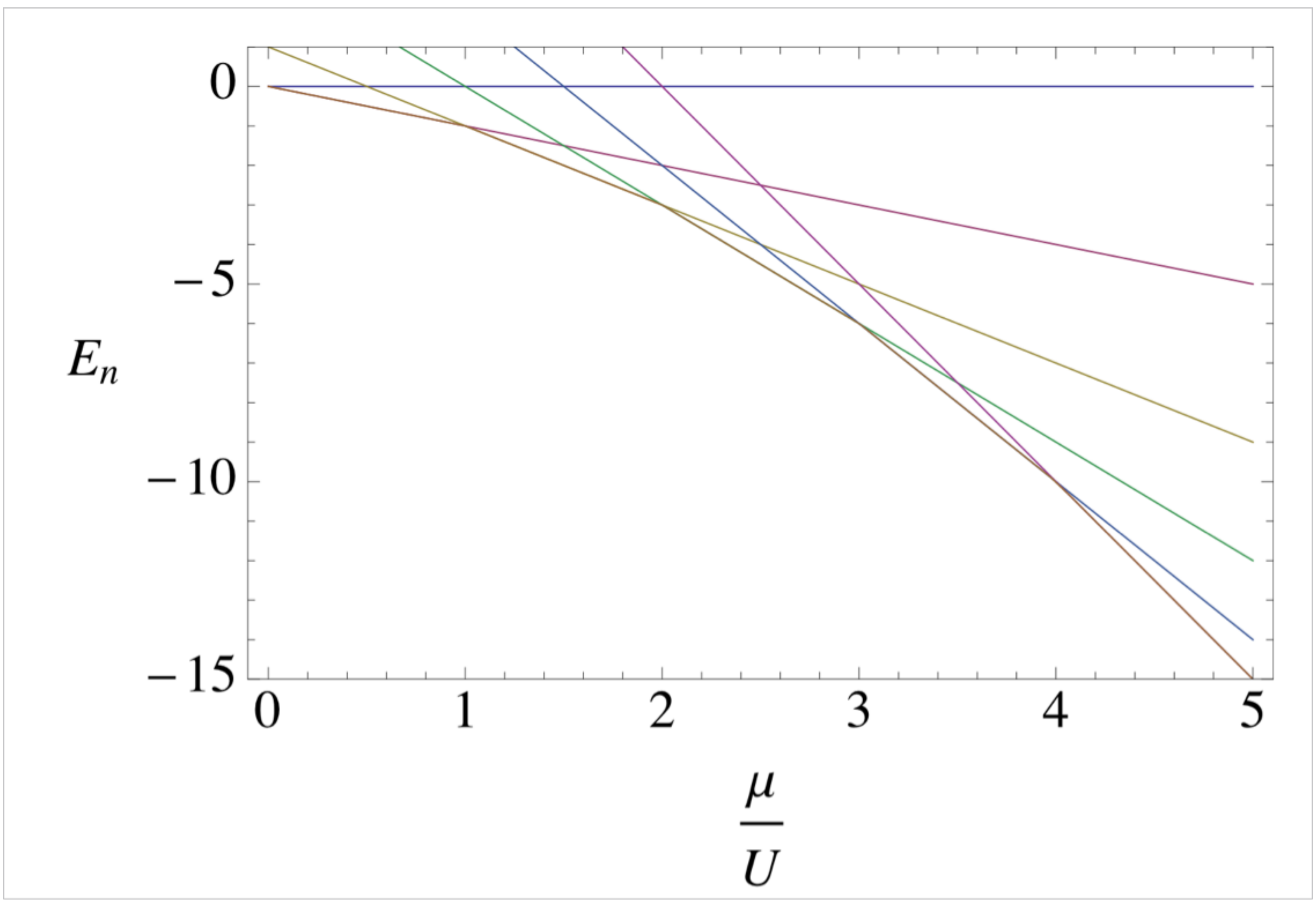
$$\tilde{\mathcal{H}}_0 |g\rangle = E_g^0 |g\rangle$$

$$E_g^0 = 0 \,, \quad \frac{\tilde{\mu}}{\tilde{U}} < 0$$

$$E_g^0 = -\frac{\tilde{\mu}}{\tilde{U}}\, g + g(g-1) \,,$$

$$\longrightarrow \quad (g-1) < \frac{\tilde{\mu}}{\tilde{U}} < g$$

Gráfica de E_g^0:



$$\tilde{q} = \left[\frac{\tilde{\mu}}{\tilde{u}} + 1 \right] ,$$

$[\cdot]$ es la parte entera.

$$E_{\tilde{q}}^{0} = -\frac{\tilde{q}\tilde{\mu}}{\tilde{u}} + \tilde{q}(\tilde{q}-1)$$

Para $\tilde{\mathcal{H}}_0$

$$V = (b + b^{+})$$

Usando Teoría de Perturbaciones

$$E_{\tilde{q}}(\varphi) = \tilde{u} E_{\tilde{q}}^{0} + \varphi^{2}$$

$$+ \varphi \langle q | V | q \rangle \leftarrow 0$$

$$+\frac{\varphi^2}{\tilde{u}}\sum_{n\neq g}\frac{|\langle g|V|n\rangle|^2}{E_g-E_n}+O(\varphi^3)$$

$$\sum_{n\neq g}\frac{|\langle g|V|n\rangle|^2}{E_g-E_n}=\frac{\tilde{g}+1}{\underline{\underline{E_g-E_{g+1}}}}+\frac{\tilde{g}}{\underline{\underline{E_g-E_{g-1}}}}$$

↳ Landau's Energy functional.

$$E_g(\varphi)=\tilde{u}E_g^0+\frac{a(\tilde{\mu},\tilde{u})}{\tilde{u}}\varphi^2+O(\varphi^3)$$

Si $a>0 \longrightarrow \varphi=0$

$a<0 \longrightarrow \varphi\neq 0$

Para minimizar $E_g(\varphi)$

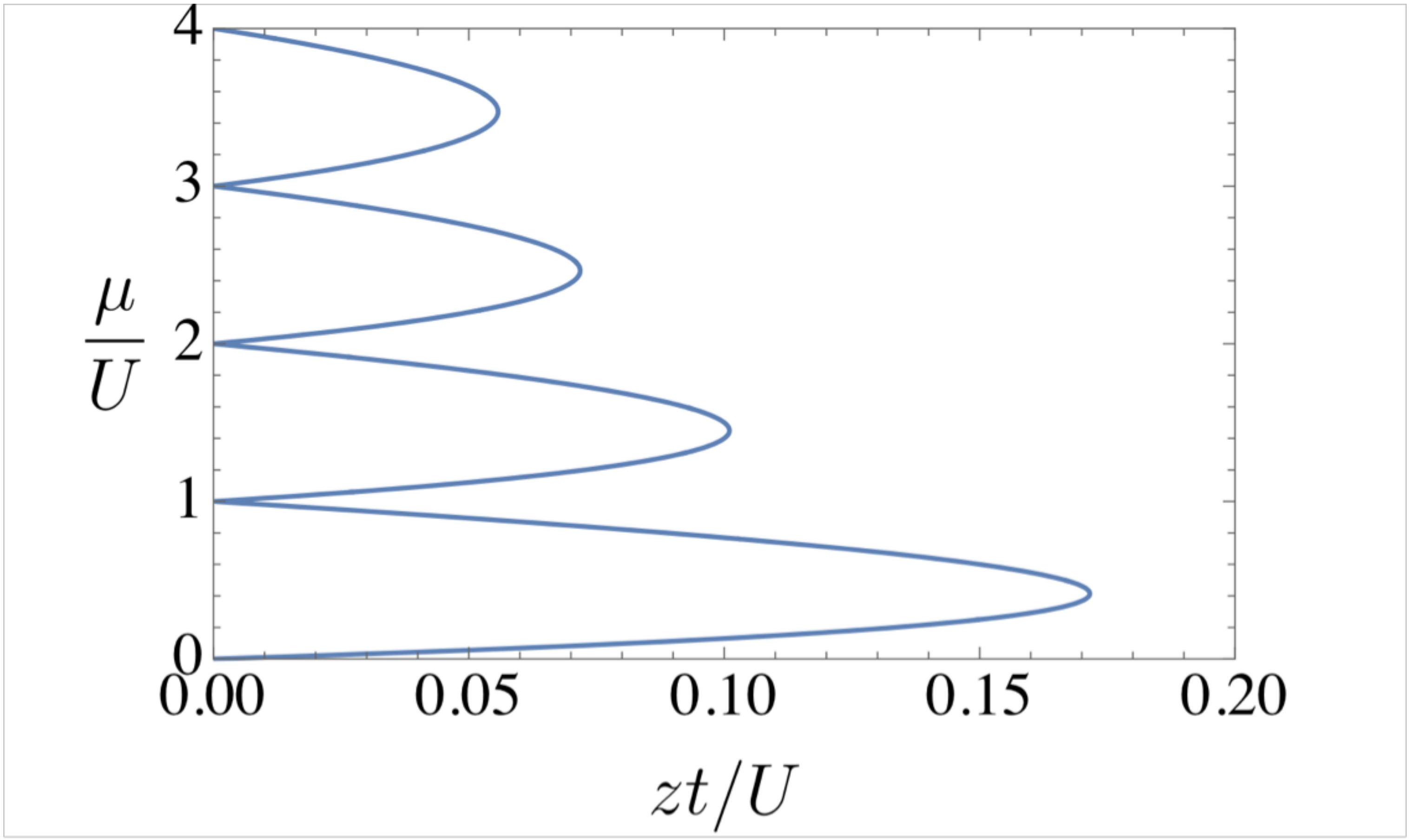
$$\therefore \quad a(\tilde{u}, \tilde{u}) \overset{!}{=} 0$$

$$= \tilde{u} + \frac{\tilde{g}+1}{\frac{\tilde{\mu}}{\tilde{u}} - \tilde{g}} + \frac{\tilde{g}}{-\frac{\tilde{\mu}}{\tilde{u}} + \tilde{g} - 1} = 0$$

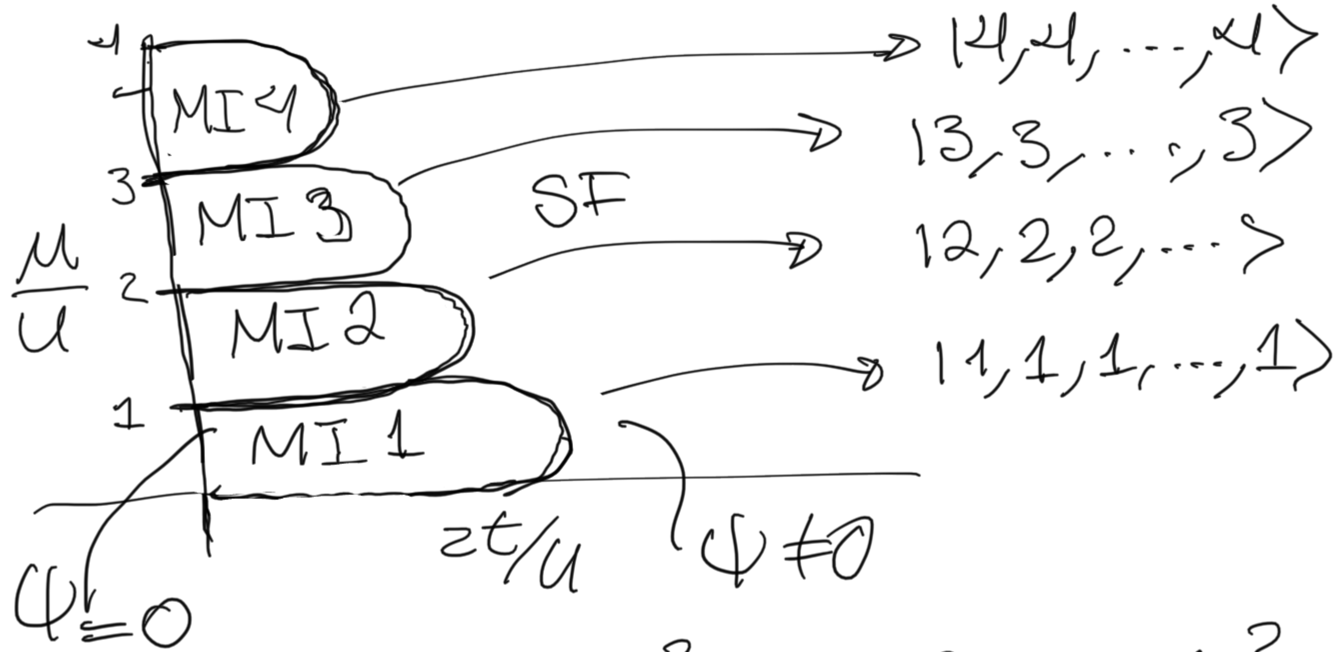
$$\boxed{y = \frac{-\tilde{g}^2 + 2x\tilde{g} + \tilde{g} - x^2 - x}{1+x}}$$

$$\boxed{\begin{aligned} y &= \frac{1}{\tilde{u}} = \frac{zt}{u} \\ x &= \frac{\tilde{\mu}}{\tilde{u}} = \frac{\mu}{u} \end{aligned}}$$

Diagrama de Fase (MFT)



4
3
$\frac{\mu}{U}$
2
1
0
0.00
0.05
0.10
0.15
0.20
zt/U



$\psi = ?$, $\Delta(\hat{n})^2 = \langle \hat{n}^2 \rangle - \langle \hat{n} \rangle^2$

$\psi \leftarrow$ $\Delta(\hat{n})^2 = 0 \leftarrow$ MI

$\Delta(\hat{n})^2 \neq 0 \leftarrow$ SF

$\downarrow$

$f_c = \mathrm{Max}\left(\frac{\lambda}{M}\right) \rightarrow$ eigenvalor de la RDM.

Implementación Numérica para encontrar el estado base y sus

propiedades. $f \to n+2$.

$$|\psi\rangle = \sum_{n=0}^{\infty} a_n |n\rangle$$

$f = 5$ (Menor a MI-3)

$$\hat{n} = \begin{pmatrix} 0 & & & & & \\ & 1 & & & & \\ & & 2 & & & \\ & & & 3 & & \\ & & & & 4 & \\ & & & & & 5 \end{pmatrix}$$

$$\hat{b} = \begin{pmatrix} 0 & & & & & \\ \sqrt{1} & 0 & & & & \\ & \sqrt{2} & 0 & & & \\ & & \sqrt{3} & 0 & & \\ & & & \sqrt{4} & 0 & \\ & & & & \sqrt{5} & 0 \end{pmatrix}$$

$\hat{b}^{\dagger} = (0 \ \sqrt{1} \ \ldots$

$$b' = \begin{pmatrix} 0 & \sqrt{2} & & & \\ & 0 & \sqrt{3} & & \\ & & 0 & \sqrt{4} & \\ & & & 0 & \sqrt{5} \\ & & & & 0 \end{pmatrix}$$

$$\tilde{\mathcal{H}} \to \dim(\tilde{\mathcal{H}}) = 6 \times 6$$

$$\underbrace{\phi(b+b^{+})}\ ,\ \phi^2 \mathbb{1}$$

$$\tilde{\mathcal{H}} \to \tilde{\mathcal{H}}(\phi)$$

1) $\phi \to \phi_0 \simeq 0.1$

2) Evalua $\tilde{\mathcal{H}}(\phi_0)$

3) Eigensystem. $\tilde{\mathcal{H}}$.

↳ Estado Base $|\phi_g\rangle$

4) $\phi = \langle \hat{b} \rangle = \langle \phi_g | \hat{b} | \phi_g \rangle$.

5) $err = |\phi - \phi_0|$

6) $\phi_0 = \phi$

7) Regresar a 2)

hasta $err < tol. \sim 10^{-3} - 10^{-5}$