FI 193 – Teoria Quântica de Sistemas de Muitos Corpos

2º Semestre de 2023

26/10/2023

Aula 21

Aula passada

Teoria de resposta linear:

$$\hat{H}_T(t) = \hat{H} + \int d^3x \varphi(\mathbf{x},t)\hat{A}(\mathbf{x}) \qquad \varphi(\mathbf{x},t) = 0 \text{ se } t < t_0$$

$$\delta\left\langle \hat{B}(\mathbf{x})\right\rangle(t) = \int d^3x' dt' D^R_{BA}(\mathbf{x}t;\mathbf{x}'t')\varphi(\mathbf{x}',t')$$

$$iD^R_{BA}(\mathbf{x}t;\mathbf{x}'t') = \theta(t-t')\langle\Psi_0|\left[\hat{B}_H(\mathbf{x},t),\hat{A}_H(\mathbf{x}',t')\right]|\Psi_0\rangle$$

Teoria de perturbação pode ser usada para calcular:

$$iD_{BA}(\mathbf{x}t;\mathbf{x}'t') = \langle\Psi_0|T\left[\hat{B}_H(\mathbf{x},t)\hat{A}_H(\mathbf{x}',t')\right]|\Psi_0\rangle$$

Aula passada

Usando a representação de Lehmann, podemos relacionar as duas quantidades:

$$D_{BA}(\mathbf{k},\omega) = V\sum_n \left[\frac{\langle\Psi_0|\hat{B}(\mathbf{0})|n\mathbf{k}\rangle\langle n\mathbf{k}|\hat{A}(\mathbf{0})|\Psi_0\rangle}{\omega-(E_n-E_0)+i\eta} - \frac{\langle\Psi_0|\hat{A}(\mathbf{0})|n\mathbf{k}\rangle\langle n\mathbf{k}|\hat{B}(\mathbf{0})|\Psi_0\rangle}{\omega+(E_n-E_0)-i\eta}\right]$$

$$D^R_{BA}(\mathbf{k},\omega) = V\sum_n \left[\frac{\langle\Psi_0|\hat{B}(\mathbf{0})|n\mathbf{k}\rangle\langle n\mathbf{k}|\hat{A}(\mathbf{0})|\Psi_0\rangle}{\omega-(E_n-E_0)+i\eta} - \frac{\langle\Psi_0|\hat{A}(\mathbf{0})|n\mathbf{k}\rangle\langle n\mathbf{k}|\hat{B}(\mathbf{0})|\Psi_0\rangle}{\omega+(E_n-E_0)+i\eta}\right]$$

$$\mathrm{Re}D^R_{BA}(\mathbf{k},\omega) = \mathrm{Re}D_{BA}(\mathbf{k},\omega)$$

$$\mathrm{Im}D^R_{BA}(\mathbf{k},\omega) = \mathrm{sgn}(\omega)\,\mathrm{Im}D_{BA}(\mathbf{k},\omega)$$

Notem que os polos nos dão as excitações criadas pela atuação de A e B no estado fundamental.

Aula passada

Uma carga estática num gás de elétrons:

$$\hat{H}_{ext}(t) = \int d^3x \varphi(\mathbf{x},t)\,\widehat{n}(\mathbf{x})\,;\ \widehat{n}(\mathbf{x}) = \sum_\sigma \psi_\sigma^\dagger(\mathbf{x})\,\psi_\sigma(\mathbf{x})$$

$$\varphi(\mathbf{x},t) = -\frac{Qe}{r} \Rightarrow \varphi(\mathbf{k},\omega) = -\frac{8\pi^2 Qe}{k^2}\delta(\omega)$$

$$\begin{aligned}
\delta\langle\widehat{n}(\mathbf{x})\rangle(t) &= \int d^3x' dt' D_{nn}^R(\mathbf{x}-\mathbf{x}', t-t')\,\varphi(\mathbf{x}',t') \\
&= \int \frac{d^3k d\omega}{(2\pi)^4} e^{i\mathbf{k}\cdot\mathbf{x}} e^{-i\omega t} D_{nn}^R(\mathbf{k},\omega)\,\varphi(\mathbf{k},\omega) \\
&= -\frac{Q}{e}\int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} D_{nn}^R(\mathbf{k},0)\left(\frac{4\pi e^2}{k^2}\right) \\
&= -\frac{Q}{e}\int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} D_{nn}^R(\mathbf{k},0)\,V(\mathbf{k})
\end{aligned}$$

Aula passada

Função de correlação carga-carga:

$$iD^{R}_{nn}\left(\mathbf{x}t;\mathbf{x}'t'\right)=\theta\left(t-t'\right)\langle\Psi_0|\left[\hat{n}_H\left(\mathbf{x},t\right),\hat{n}_H\left(\mathbf{x}',t'\right)\right]|\Psi_0\rangle$$

$$\widetilde{n}\left(\mathbf{x}\right)=\widehat{n}\left(\mathbf{x}\right)-n \quad \Rightarrow D^{R}_{nn}\left(\mathbf{x}t;\mathbf{x}'t'\right)=D^{R}_{\widetilde{n}\widetilde{n}}\left(\mathbf{x}t;\mathbf{x}'t'\right)$$

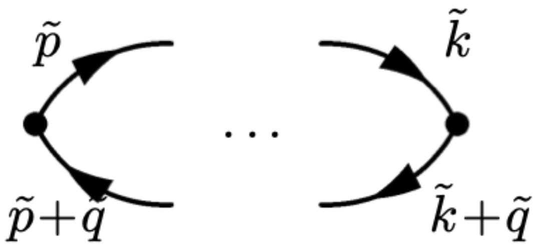
A função de correlação ordenada temporalmente:

$$\begin{aligned}
iD_{\widetilde{n}\widetilde{n}}\left(\mathbf{x}t;\mathbf{x}'t'\right) &= \langle\Psi_0|T\left[\widetilde{n}_H\left(\mathbf{x},t\right)\widetilde{n}_H\left(\mathbf{x}',t'\right)\right]|\Psi_0\rangle \\
&= \underbrace{\langle\Psi_0|T\left[n_H\left(\mathbf{x},t\right)n_H\left(\mathbf{x}',t'\right)\right]|\Psi_0\rangle}_{iD_{nn}(\bar{x}t;\,\bar{x}'t')}-n^2
\end{aligned}$$

$$\begin{aligned}
iD_{nn}\left(\mathbf{x}t;\mathbf{x}'t'\right) &= \langle\Psi_0|T\left[n_H\left(\mathbf{x},t\right)n_H\left(\mathbf{x}',t'\right)\right]|\Psi_0\rangle \\
&= \frac{\langle\Phi_0|T\left[\tilde{U}\left(+\infty,-\infty\right)n_I\left(\mathbf{x},t\right)n_I\left(\mathbf{x}',t'\right)\right]|\Phi_0\rangle}{\langle\Phi_0|\tilde{U}\left(+\infty,-\infty\right)|\Phi_0\rangle}
\end{aligned}$$

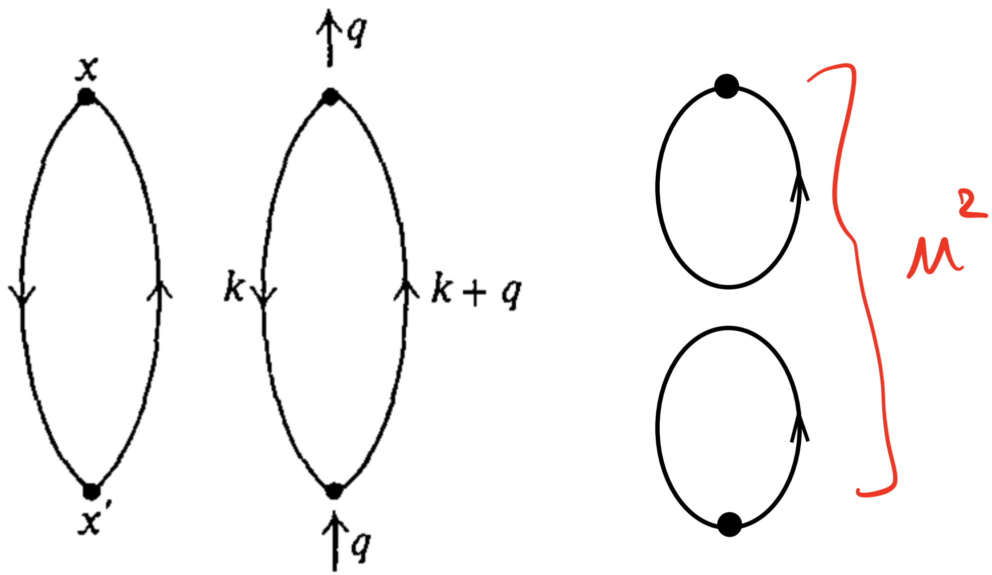
Função de correlação carga-carga

$$iD_{nn}(\mathbf{x}t;\mathbf{x}'t') = \frac{\langle\Phi_0|\,T\left[\tilde{U}(+\infty,-\infty)\,\psi^\dagger_{\alpha I}(\mathbf{x},t)\,\psi_{\alpha I}(\mathbf{x},t)\,\psi^\dagger_{\beta I}(\mathbf{x}',t')\,\psi_{\beta I}(\mathbf{x}',t')\right]|\Phi_0\rangle}{\langle\Phi_0|\,\tilde{U}(+\infty,-\infty)\,|\Phi_0\rangle}$$



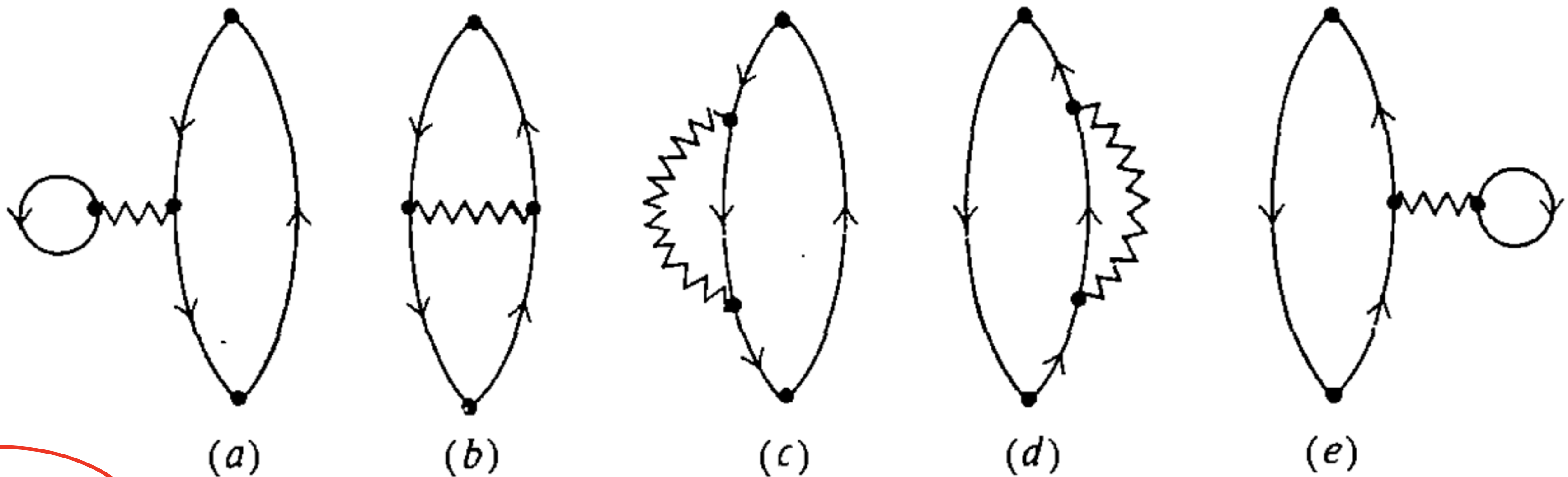
$D^{(0)}_{nn}(x-x')$

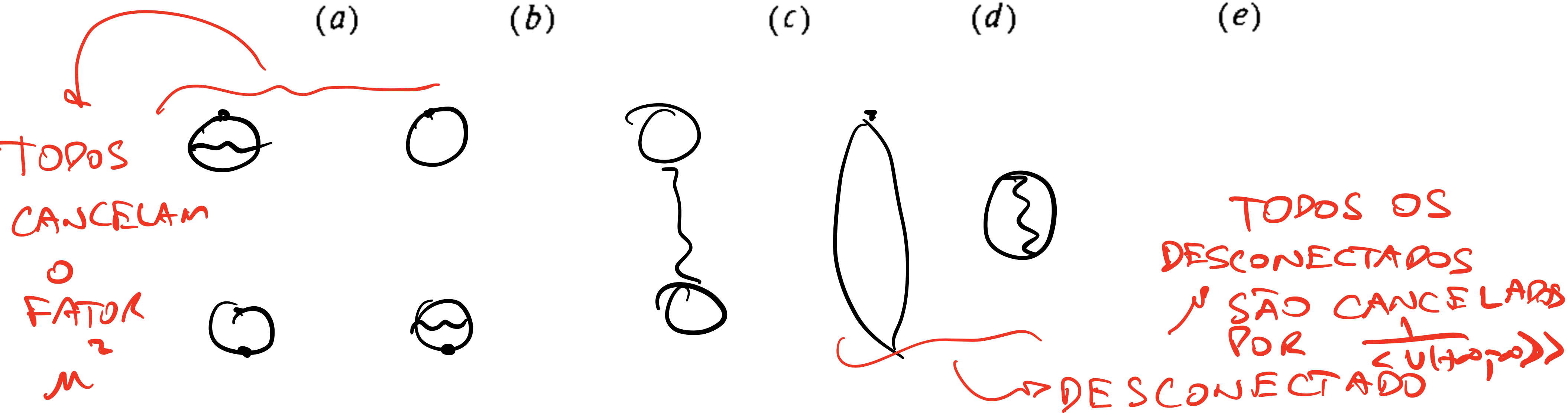
Em ordem zero:



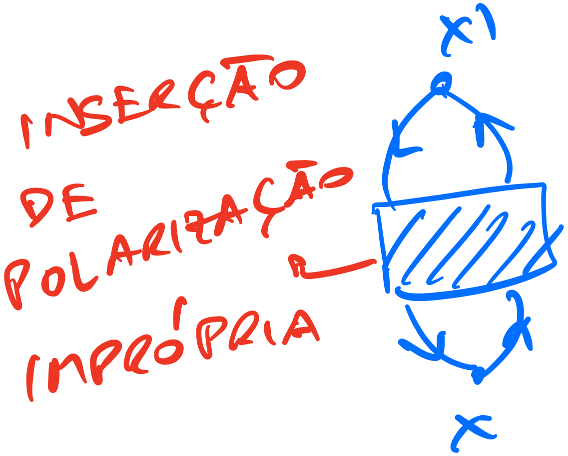
Função de correlação carga-carga

Em ordens superiores: EM ORDEM 1





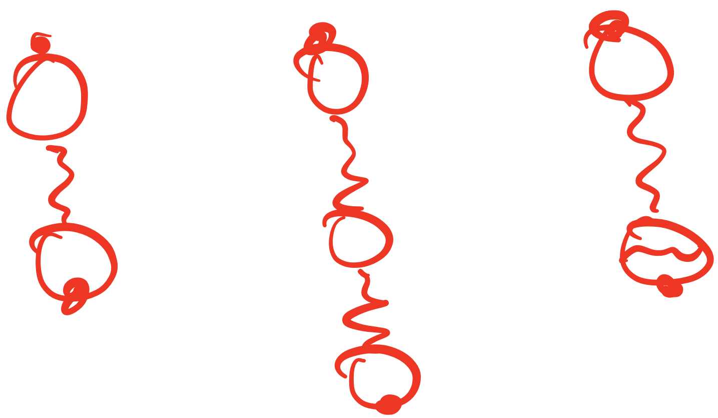
TODOS OS DIAGRAMAS DE $D_{\tilde{n}\tilde{n}}(x-x')$ TÊM A FORMA GERAL:



$$\Rightarrow \not{i}\, D_{\tilde{n}\tilde{n}}(x-x') = \not{i}\, \tilde{\Pi}(x-x')$$

$$\Rightarrow \boxed{D_{\tilde{n}\tilde{n}}(x-x') = \tilde{\Pi}(x-x')}$$

TEM QUE SER A IMPRÓPRIA PORQUE DIAGRAMAS COMO



ESTÃO INCLUÍDOS

MAS: $\tilde{\Pi}(q) = \dfrac{\Pi(q)}{1 - V(q)\Pi(q)}$ ONDE $\Pi(q)$ É A INSERÇÃO DE POLARIZAÇÃO PRÓPRIA.

$$D^R(\vec{k},0)V(\vec{k}) = ?$$

$$D(k) = \frac{\Pi(k)}{1 - V(\vec{k})\Pi(k)} \longrightarrow D^R(k) = \frac{\Pi^R(k)}{1 - V(\vec{k})\Pi^R(k)}$$

MAS EU PRECISO DE $D^R(\vec{k},0)$:

$$D^R(\vec{k},0) = \frac{\Pi^R(\vec{k},0)}{1 - V(\vec{k})\Pi^R(\vec{k},0)}$$

MAS, NO LIMITE DE ALTAS DENSIDADES, $\Pi(k) \simeq \Pi^{(0)}(k)$

E: $\Pi^{(0)}(\vec{k},0) = -\frac{m k_F}{\pi^2} g(k/k_F) \in \mathbb{R}$ $\qquad \frac{m k_F}{\pi^2} = \rho_F$

ONDE:

$$g(x) = \frac{1}{2} - \frac{1}{2x}\left(1 - \frac{x^2}{4}\right) \ln\left|\frac{1 - x/2}{1 + x/2}\right|$$

NOTE QUE $g(x)$ É NÃO ANALÍTICA EM $x = 2$

$\Rightarrow k = 2k_F$

$$\delta\langle\hat{n}(\vec{x})\rangle = -\frac{Q}{e}\int\frac{d^3k}{(2\pi)^3}\,e^{i\vec{k}\cdot\vec{x}}\,D^R_{\tilde{n}\tilde{n}}(\vec{k},0)\,V(\vec{k})$$

$$= -\frac{Q}{e}\int\frac{d^3k}{(2\pi)^3}\,e^{i\vec{k}\cdot\vec{x}}\,\frac{\Pi^{(0)}(\vec{k},0)\,V(\vec{k})}{1-\Pi^{(0)}(\vec{k},0)V(\vec{k})}$$

$$\boxed{\delta\langle\hat{n}(\vec{x})\rangle = \frac{Q}{e}\int\frac{d^3k}{(2\pi)^3}\,e^{i\vec{k}\cdot\vec{x}}\,\frac{(4\alpha r_s/\pi)\,g(k/k_F)}{\left(\frac{k}{k_F}\right)^2+\frac{4\alpha r_s}{\pi}\,g(k/k_F)}}$$

$$\alpha = \left(\frac{4}{9\pi}\right)^{1/3}$$

(i) $\int\delta\langle\hat{n}(\vec{x})\rangle = -Q$

A CARGA INDUZIDA PELA PERTURBAÇÃO BLINDA COMPLETAMENTE A CARGA INSERIDA.

(ii) INGENUAMENTE, SE $|\vec{x}|\to\infty$, BASTARIA TOMAR O INTEGRANDO EM $|\vec{k}|=0$, $g(0)=1$

$$\delta\langle\hat{n}(\vec{x})\rangle \simeq \frac{q_{TF}^2}{4\pi x}\,e^{-q_{TF}x}$$

q_{TF} = VETOR DE ONDA DE THOMAS-FERMI

(iii) NA VERDADE, DEVIDO À NÃO-ANALITICIDADE DE $g(x)$ EM $x = 2$, O COMPORTAMENTO ASSINTÓTICO NÃO É EXPONENCIAL: (F+W; Pgs. 178-180)

$$\delta\langle \hat{n}(\vec{x})\rangle \cong -\frac{2\xi/\pi}{4+\xi}\,\frac{\cos(2k_F x)}{x^3}$$ → OSCILAÇÕES DE FRIEDEL

ONDE: $\xi = \dfrac{g_{TF}^2}{2k_F^2}$

- EM D-DIMENSÕES: $\delta n \sim \dfrac{1}{x^D}$

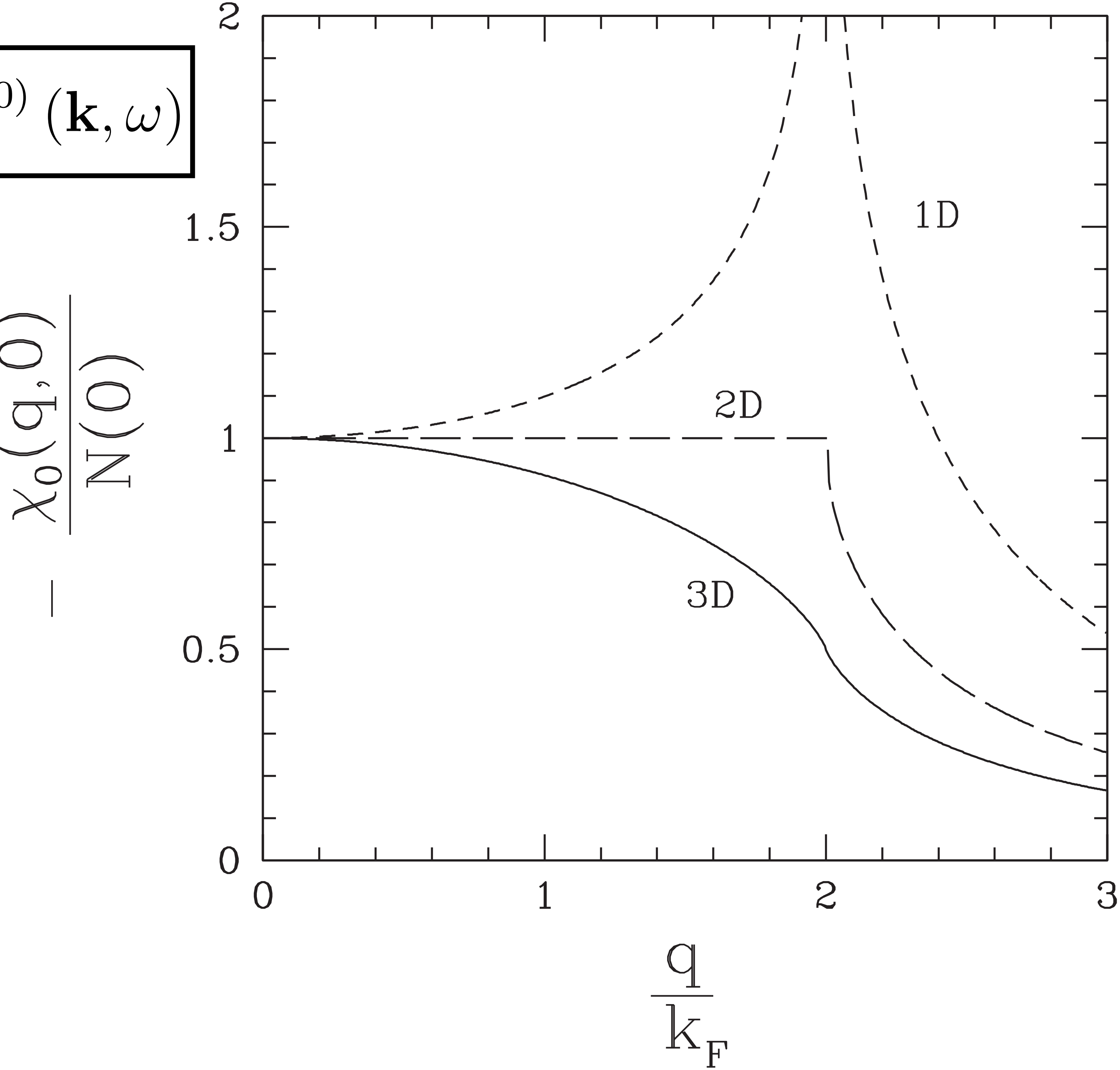
- VETOR DE ONDA DA OSCILAÇÃO, $2k_F$, GENERALIZA-SE, PARA SUPERFÍCIES DE FERMI MAIS COMPLICADAS COMO SENDO OS DIÂMETROS EXTREMAIS DA S.F. PARA CORTES PERPENDICULARES À DIREÇÃO DE $\vec{x}$.

$$\boxed{\chi_0(\mathbf{k},\omega) \equiv \pi^{(0)}(\mathbf{k},\omega)}$$

$$\bar{q}_\sigma = \frac{q}{k_{F\sigma}}.$$

d	$\chi_{0\sigma}(q,0)$
3	$-N_\sigma(0)\left[\frac{1}{2} + \frac{\bar{q}_\sigma^2 - 4}{8\bar{q}_\sigma} \ln\left\|\frac{\bar{q}_\sigma - 2}{\bar{q}_\sigma + 2}\right\|\right]$
2	$-N_\sigma(0)\left[1 - \Theta(\bar{q}_\sigma - 2)\frac{\sqrt{\bar{q}_\sigma^2 - 4}}{\bar{q}_\sigma}\right]$
1	$-N_\sigma(0)\left[\frac{1}{\bar{q}_\sigma} \ln\left\|\frac{\bar{q}_\sigma + 2}{\bar{q}_\sigma - 2}\right\|\right]$

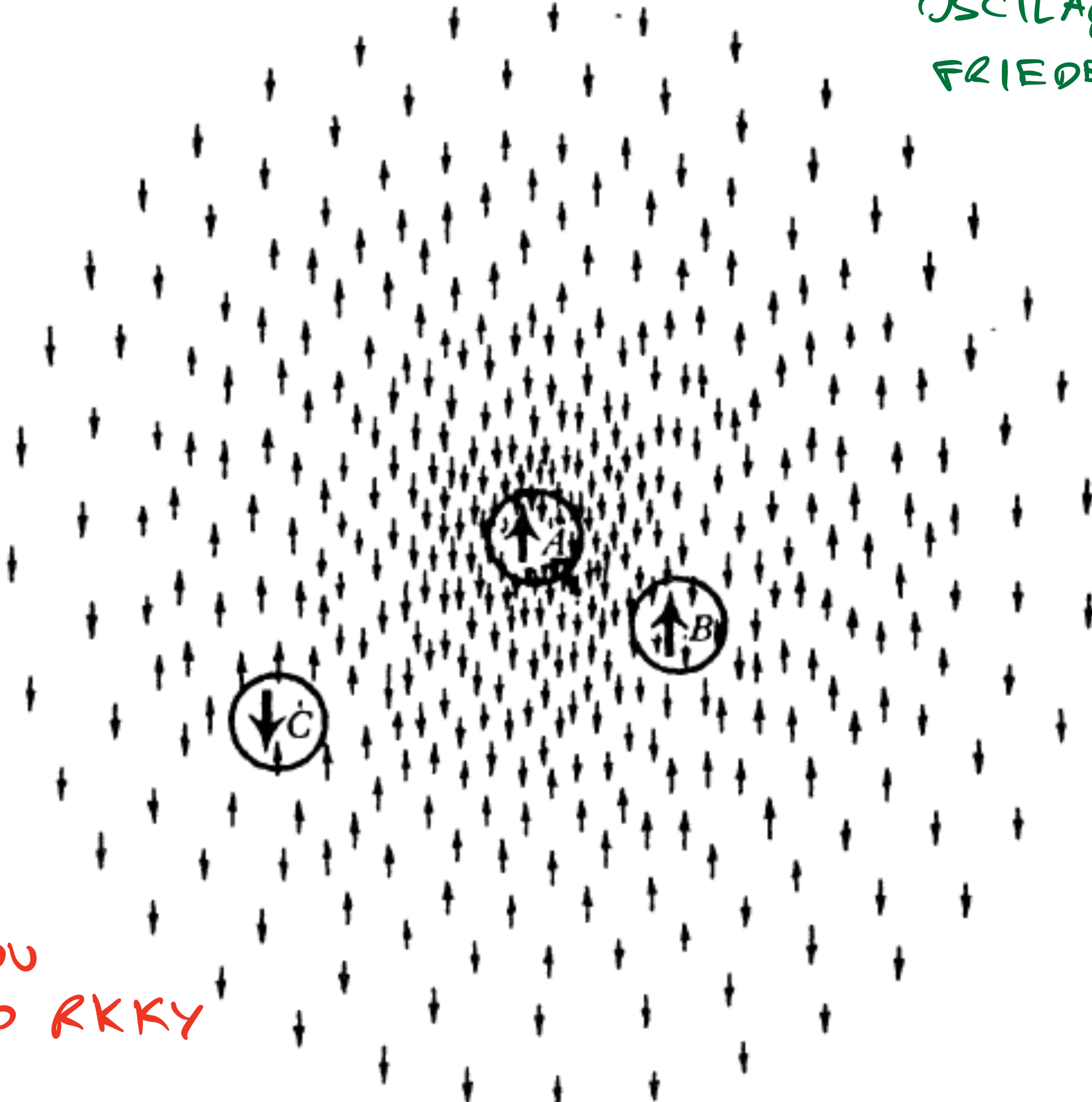
$$\chi_0(\mathbf{k},\omega) \equiv \pi^{(0)}(\mathbf{k},\omega)$$



$$\boxed{\chi_0(\mathbf{r},0) \equiv \pi^{(0)}(\mathbf{r},0)}$$

d	$\chi_{0\sigma}(r,0)$
3	$12\pi n_\sigma N_\sigma(0)\frac{\sin 2k_{F\sigma}r - 2k_{F\sigma}r\cos 2k_{F\sigma}r}{(2k_{F\sigma}r)^4}$
2	$2\pi n_\sigma N_\sigma(0)\left[J_0(k_{F\sigma}r)N_0(k_{F\sigma}r) + J_1(k_{F\sigma}r)N_1(k_{F\sigma}r)\right]$
1	$\pi n_\sigma N_\sigma(0)\,\mathrm{si}(2k_{F\sigma}x)$

OSCILAÇÕES DE FRIEDEL DE SPIN



EXCHANGE INDIRETO OU INTERAÇÃO RKKY

A POLARIZAÇÃO INDUZIDA GERA ACOPLAMENTO ENTRE SPINS LOCALIZADOS (A,B,C)

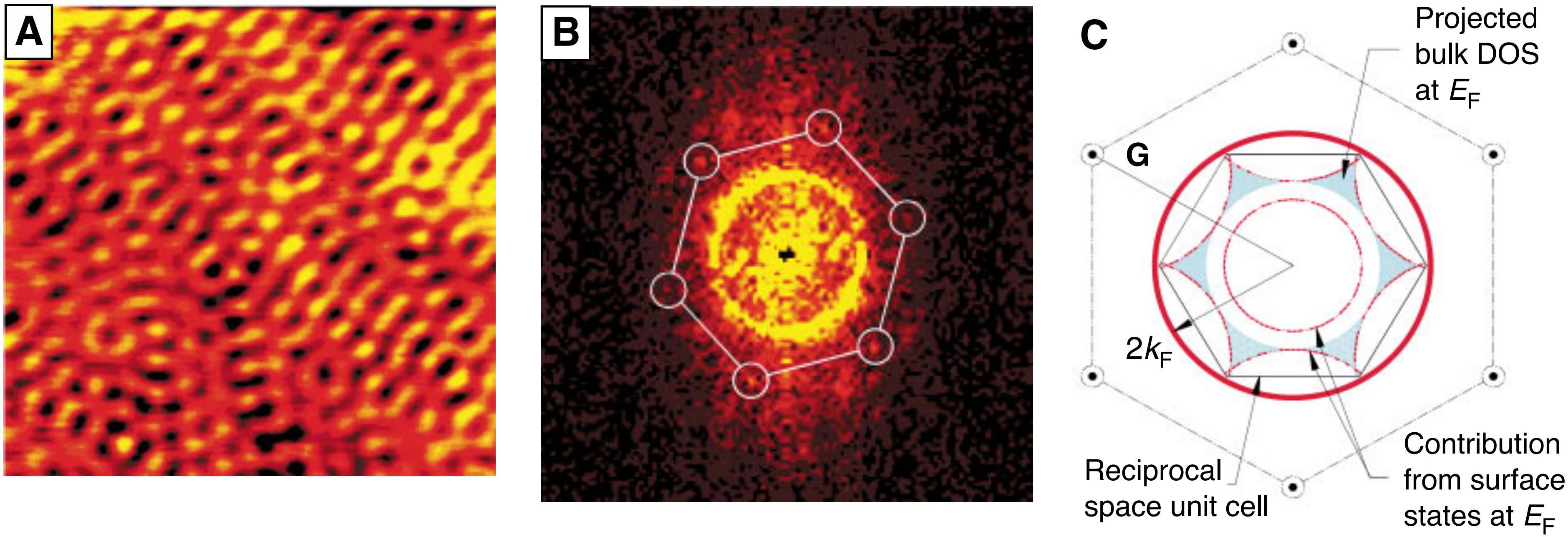


Fig. 2. (**A**) Constant-current STM image (40 Å by 40 Å, $I = 1.5$ nA, $V = 4$ mV) of Be(0001) at 150 K. (**B**) The 2D FT of the image in (A). (**C**) The 2D Brillouin zone of Be(0001) in which the circles (shaded region) correspond to the surface states (projected bulk bands) at E_F. The reciprocal space unit cell with the corresponding $2k_F$ "ring" is also shown.

(A) Imagem crua obtida com STM da superfície Be(0001)

(B) Transformada de Fourier de (A) mostrando $2k_F$ dos estados de superfície (círculo menor do painel (C)).

(C) Superfície de Fermi 2D (bulk e superfície).

P. T. Sprunger, L. Petersen, E. W. Plummer, E. Lægsgaard, F. Besenbacher, Science **275**, 1764 (1997).

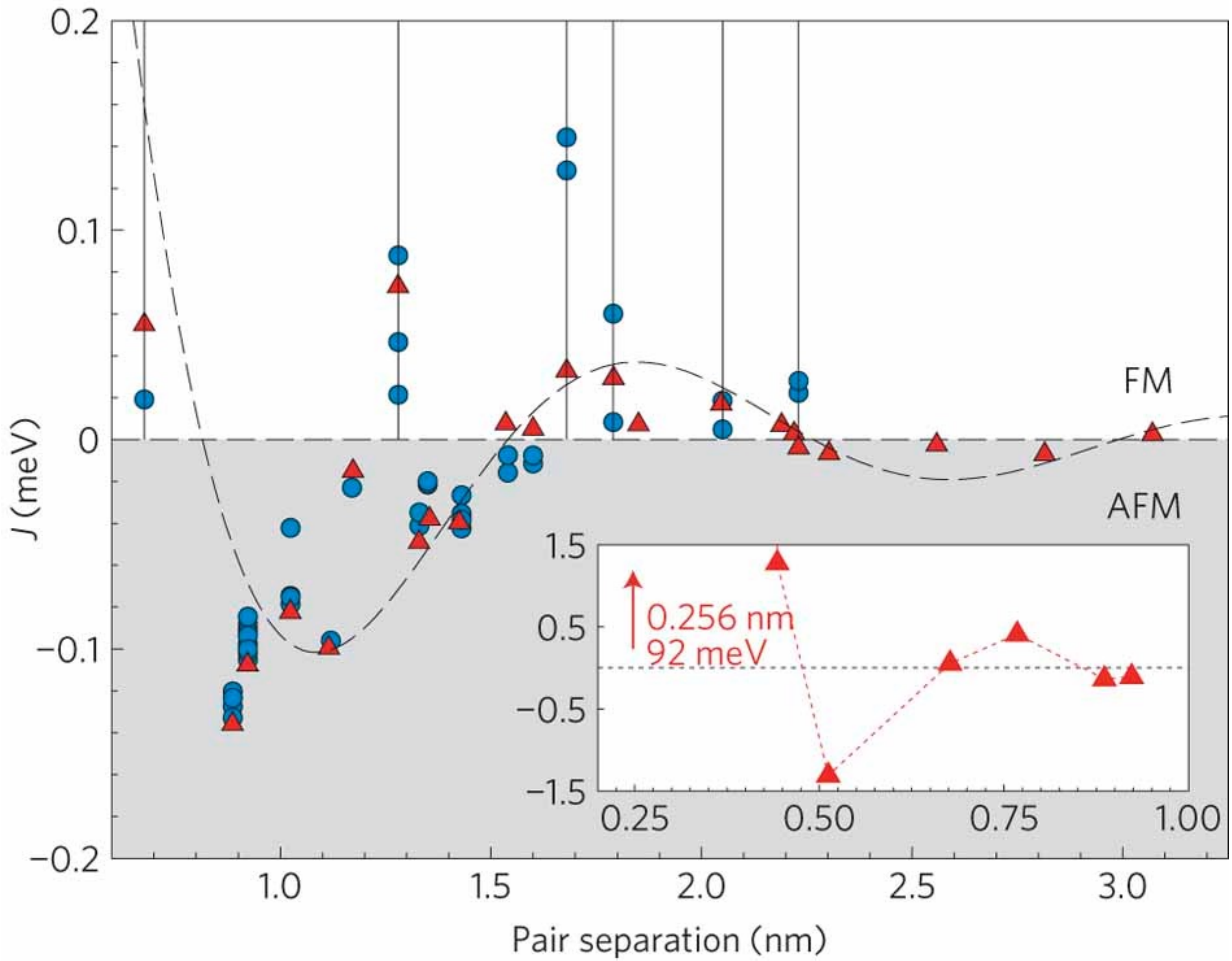


Figure 1 | Distance dependency of pairwise RKKY interaction energy. Measured (blue circles) and KKR-calculated (red triangles, renormalized by a factor of 1/2) exchange energy J_{ij} in pairs of Fe atoms on Cu(111) as a function of separation. The dashed line indicates a fit of the AFM experimental data to a sinusoidal RKKY model, taking into account the Fermi wavelength of the Cu(111) surface state. The inset shows the renormalized KKR-calculated values for closer separations.

A. A. Khajetoorians, J. Wiebe, B. Chilian, S. Lounis, S. Blügel & R. Wiesendanger, Nature Physics **8**, 497–503 (2012)

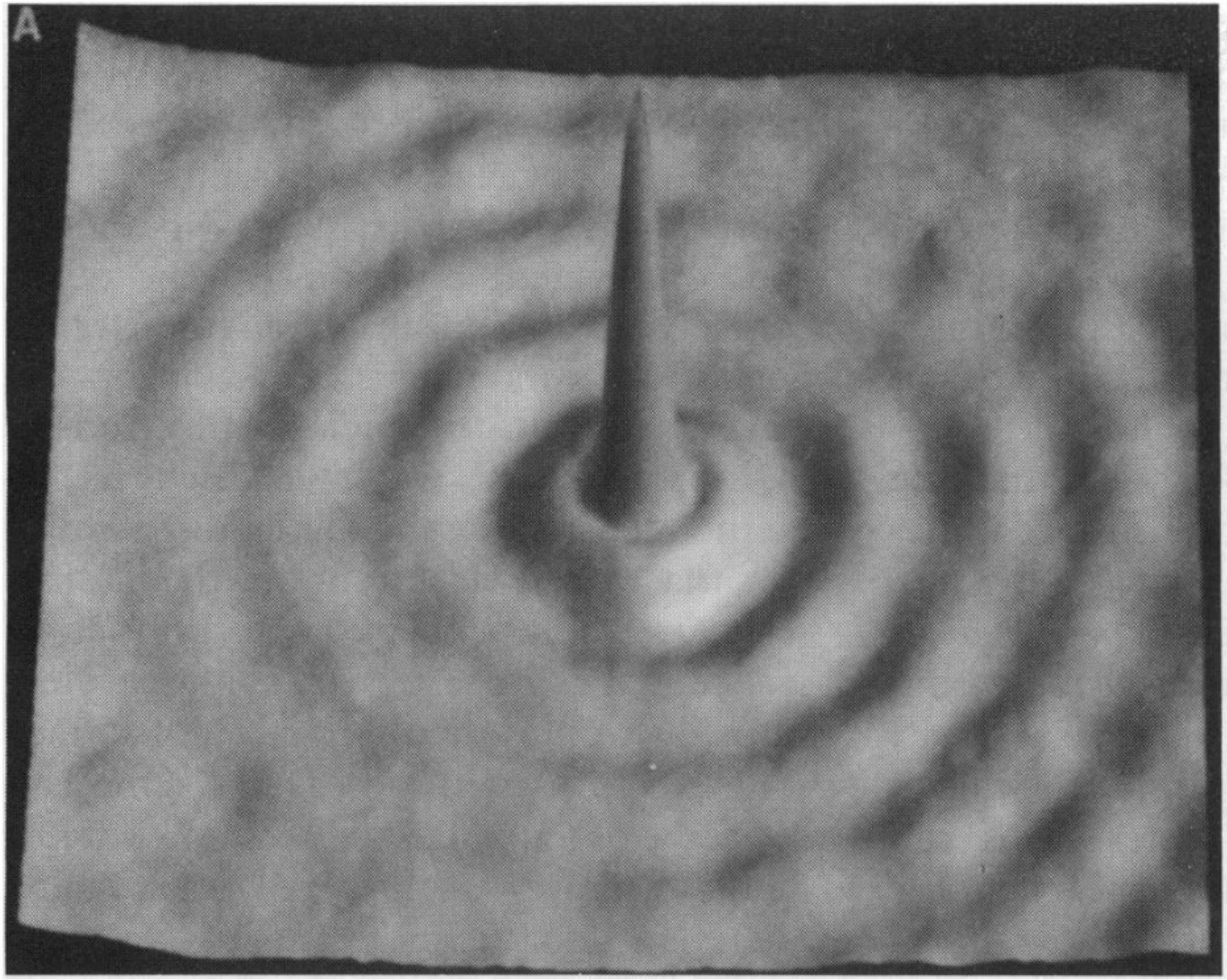
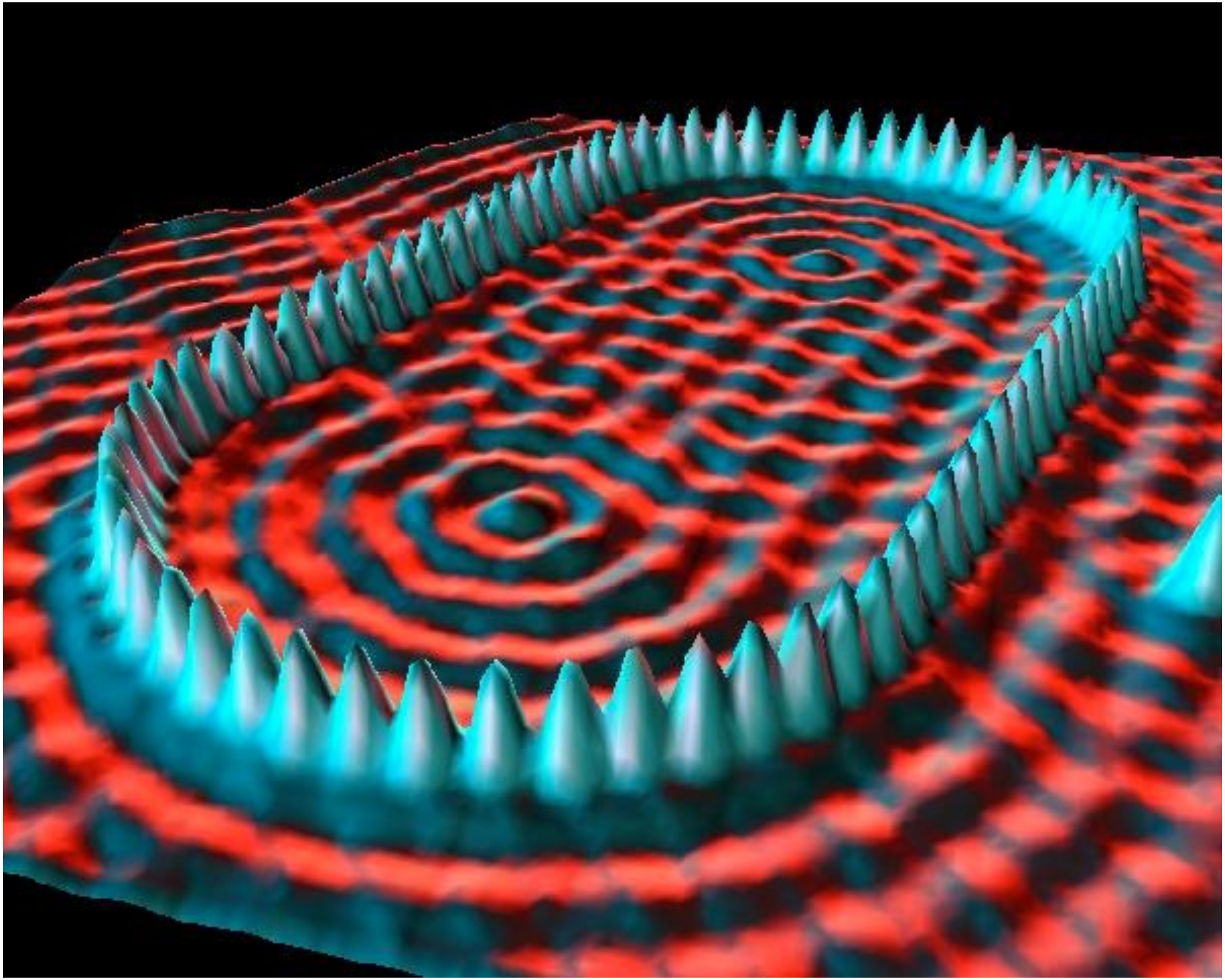


Fig. 1. **(A)** Constant current 130 Å × 130 Å image of an Fe adatom on the Cu(111) surface (V = 0.02 volt, I = 1.0 nA). The apparent height of the adatom is ~0.9 Å. The concentric rings surrounding the Fe adatom are standing waves due to the scattering of surface state electrons with

M. F. Crommie, C. P. Lutz, D. M. Eigler, Science **262**, 218 (1993)

Curral quântico



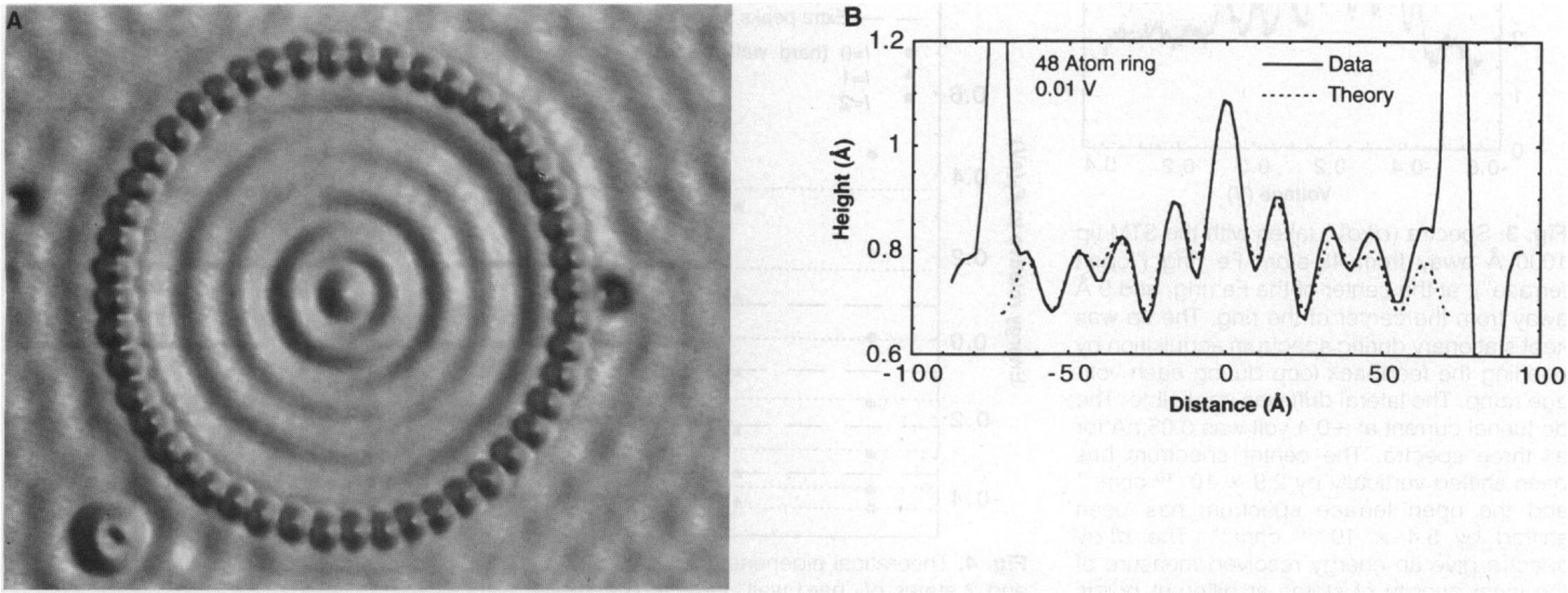


Fig. 2. Spatial image of the eigenstates of a quantum corral. (**A**) 48-atom Fe ring constructed on the Cu(111) surface ($V = 0.01$ volt, $I = 1.0$ nA). Average diameter of ring (atom center to atom center) is 142.6 Å. The ring encloses a defect-free region of the surface. (**B**) Solid line: cross section of the above data. Dashed line: fit to cross section using a linear combination of $|5,0\rangle$, $|4,2\rangle$, and $|2,7\rangle$ eigenstate densities.

M. F. Crommie, C. P. Lutz, D. M. Eigler, Science **262**, 218 (1993)

Resumindo

$$D_{nn}(\mathbf{k},\omega) = \tilde{\pi}(\mathbf{k},\omega) = \frac{\pi(\mathbf{k},\omega)}{1 - V(\mathbf{k})\,\pi(\mathbf{k},\omega)}$$

$$D_{nn}(\mathbf{k},\omega) \approx \frac{\pi^{(0)}(\mathbf{k},\omega)}{1 - V(\mathbf{k})\,\pi^{(0)}(\mathbf{k},\omega)} \text{ se } r_s \ll 1$$

Da representação de Lehmann:

$$D_{nn}(\mathbf{k},\omega) = V\sum_n \left[\frac{\langle\Psi_0|\,\hat{n}(-\mathbf{k})\,|n\mathbf{k}\rangle\,\langle n\mathbf{k}|\,\hat{n}(\mathbf{k})\,|\Psi_0\rangle}{\omega - (E_n - E_0) + i\eta} - \frac{\langle\Psi_0|\,\hat{n}(\mathbf{k})\,|n\mathbf{k}\rangle\,\langle n\mathbf{k}|\,\hat{n}(-\mathbf{k})\,|\Psi_0\rangle}{\omega + (E_n - E_0) - i\eta}\right]$$

$$D^R_{nn}(\mathbf{k},\omega) = V\sum_n \left[\frac{\langle\Psi_0|\,\hat{n}(-\mathbf{k})\,|n\mathbf{k}\rangle\,\langle n\mathbf{k}|\,\hat{n}(\mathbf{k})\,|\Psi_0\rangle}{\omega - (E_n - E_0) + i\eta} - \frac{\langle\Psi_0|\,\hat{n}(\mathbf{k})\,|n\mathbf{k}\rangle\,\langle n\mathbf{k}|\,\hat{n}(-\mathbf{k})\,|\Psi_0\rangle}{\omega + (E_n - E_0) + i\eta}\right]$$

Estrutura de polos da função de correlação densidade-densidade

$$\pi^{(0)R}(q) = 2\int \frac{d^3k}{(2\pi)^3}\left[\frac{\theta(k_F - k)\,\theta(|\mathbf{k}+\mathbf{q}| - k_F)}{\nu + \epsilon(\mathbf{k}) - \epsilon(\mathbf{k}+\mathbf{q}) + i\eta} - \frac{\theta(k - k_F)\,\theta(k_F - |\mathbf{k}+\mathbf{q}|)}{\nu + \epsilon(\mathbf{k}) - \epsilon(\mathbf{k}+\mathbf{q}) + i\eta}\right]$$

BURACO ELÉTRON ELÉTRON BURACO

$$\nu = \epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} = \frac{q^2}{2m} + \frac{\mathbf{k}\cdot\mathbf{q}}{m}; \quad \begin{cases} k < k_F \quad \text{e} \quad |\mathbf{k}+\mathbf{q}| > k_F \\ \qquad \text{ou} \\ k > k_F \quad \text{e} \quad |\mathbf{k}+\mathbf{q}| < k_F \end{cases}$$

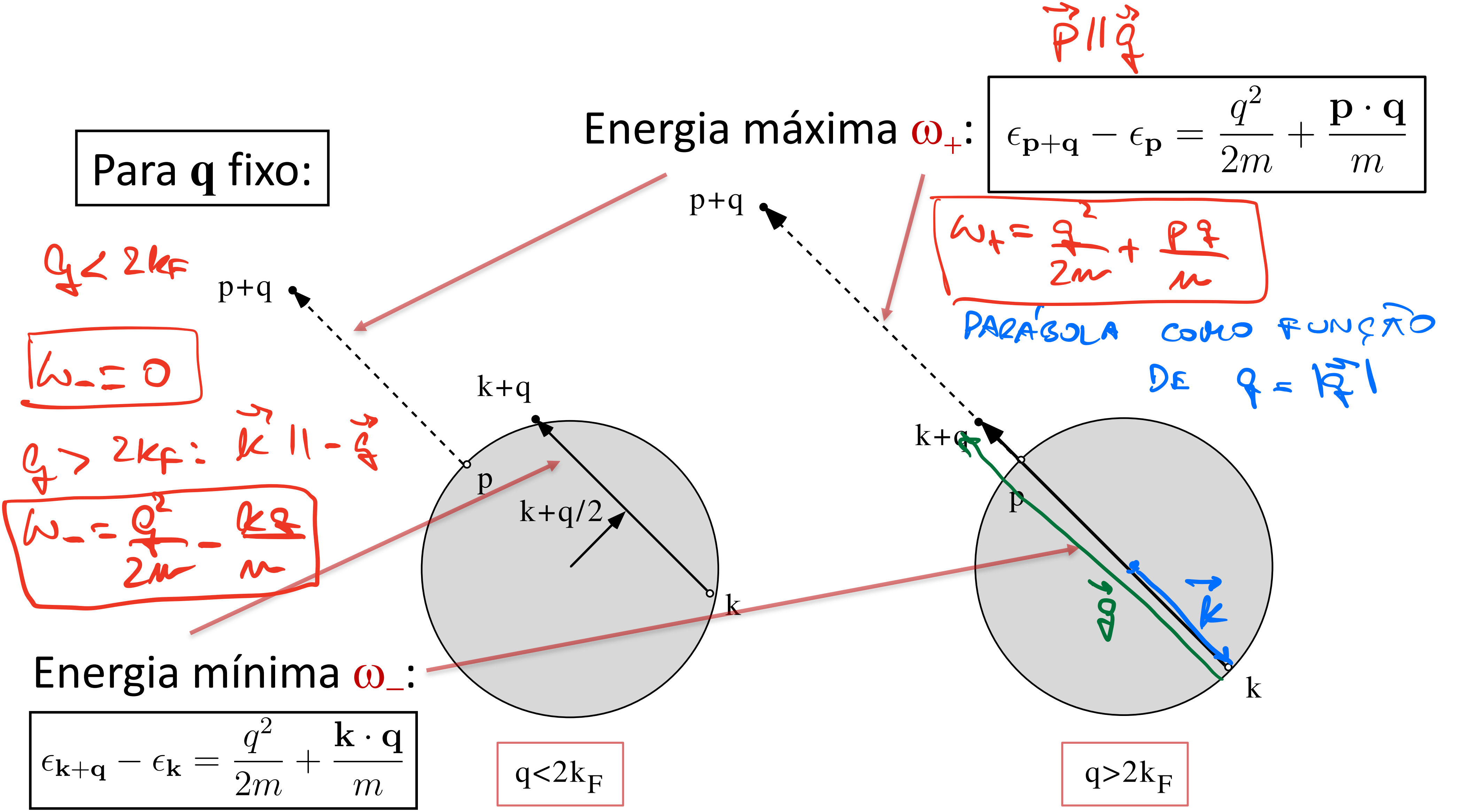
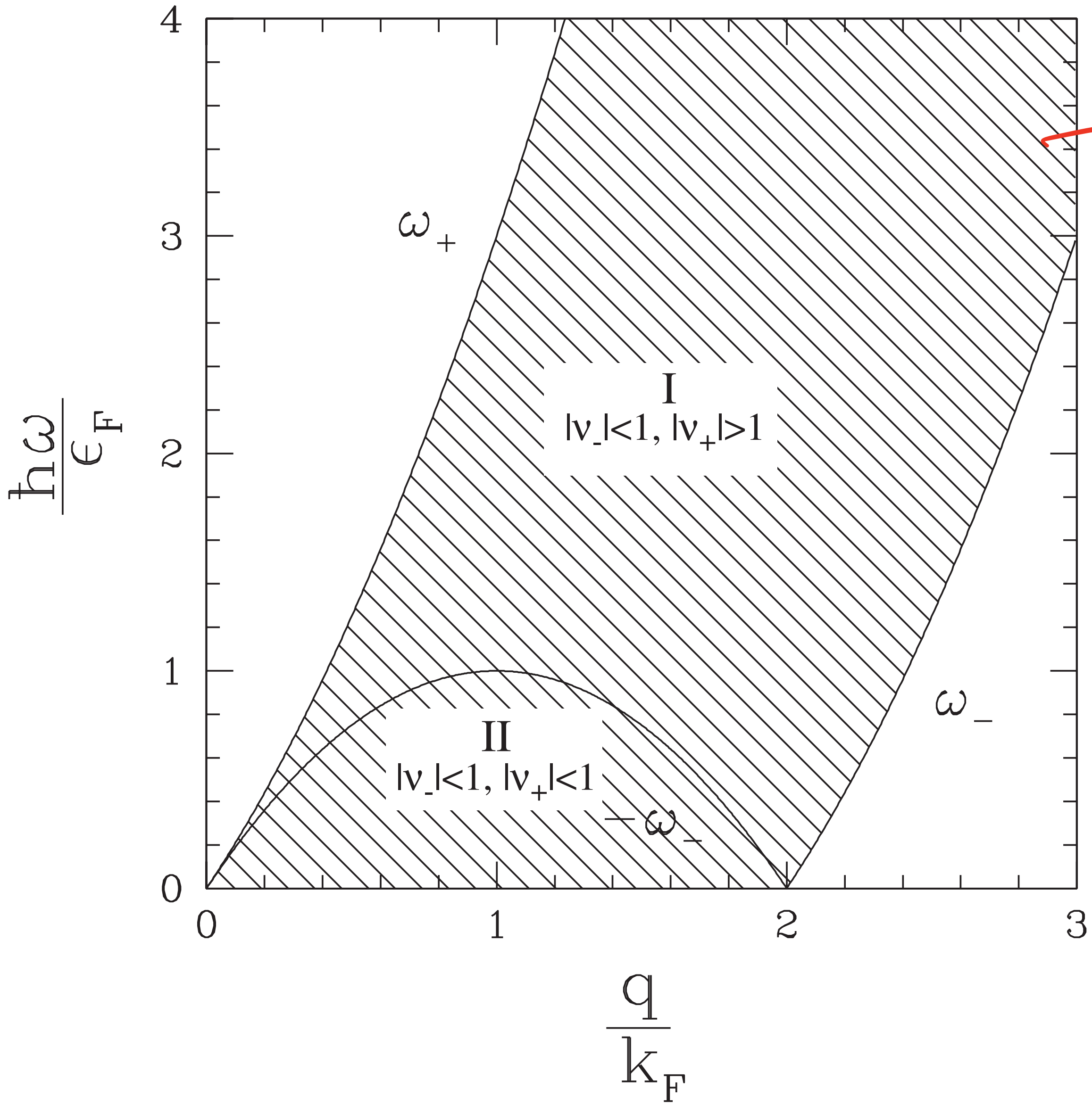


Fig. 4.3. electron–hole pairs of minimum energy ($\vec{k} \rightarrow \vec{k} + \vec{q}$ – solid line) and maximum energy ($\vec{p} \rightarrow \vec{p} + \vec{q}$ – dashed line) for a given wave vector $\vec{q}$. Notice that for zero energy excitations the sum of the initial and final wave vectors, that is, $2\left(\vec{k} + \frac{\vec{q}}{2}\right)$, is orthogonal to $\vec{q}$.



CONTÍNUO DE EXCITAÇÕES PARTÍCULA-BURACO

$$\max(0, \omega_-(q)) \leq |\omega| \leq \omega_+(q)$$

$$\omega_\pm(q) = \frac{\hbar q^2}{2m} \pm v_F q$$

A região II está ausente em uma dimensão!