CLASSIFYING VARIATIONAL FUNCTIONS FOR QUASI-ONE-DIMENSIONAL
SYSTEMS AND INCORPORATING ELECTRON CORRELATION

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A classification is proposed for the variation functions in the variable local-
ized geminals (VLG) approximation based on the types of variational function in
the unrestricted Hartree-Fock (UHF) method for one-dimensional systems. It has
been found that functions of VLG type provide better incorporation of electron-
correlation effects than do UHF ones. A study has been made on the phase dia-
gram for the electronic states of polyacetylene in relation to the electron-
electron parameters in the extrended Hubbard Hamiltonian containing certain types
of VLG function.

Various theoretical approaches have been used [1-9] in research on one-dimensional con-
jugated systems in order to give fuller incorporation of electron Coulom-interaction correlation
effects. Here the generalized Hartree—Fock method (GHFM) and the variable localized geminal
(VLG) method incorporate configuration interaction incompletely but can be applied effec-
tively to more extended systems. Here we use ideas from [8] in new variational functions,
whose performance is discussed in describing polyene chain features.

VLG FUNCTION CLASSIFICATION

The following form can be given for the variational wave function for the ground state
of the π electrons in a cyclic polyene $(CH)_{2M}$ (with one π electron in each atomic carbon
$2p_z$ orbital):

$$\Phi = \prod_{m=1}^{M} g_m^+ |0\rangle, \tag{1}$$

$$g_m^+ = u f_{m1/2\alpha}^+ f_{m1/2\beta}^+ + v f_{m-1/2\alpha}^+ f_{m-1/2\beta}^+ + w (f_{m1/2\alpha}^+ f_{m-1/2\beta}^+ + f_{m1/2\beta}^+ f_{m-1/2\alpha}^+),$$

$$u^2 + 2w^2 + v^2 = 1, \tag{2}$$

where g_m^+ is the operator for electron-pair generation in a geminal localized on atomic pair
m, $f_{m\alpha\sigma}^+$ is the operator for electron generation in one of the two one-electron $(\alpha = \pm 1/2)$
states localized on pair m with spin σ ($\sigma = +1/2$ or $-1/2$, which is denoted by the subscripts
α and β). The operators $f_{m\alpha\sigma}^+$ $(f_{m\alpha\sigma})$ are expressed in terms of the corresponding ones for an
electron in AO n $c_{n\sigma}^+$ $(c_{n\sigma})$ and in MO $a_{k\sigma}^+$ $(a_{k\sigma})$ having quasimomentum k:

$$f_{m\alpha\sigma} = \sum_{|k|<k_F} U_{mk} \varphi_{ak\sigma}, \tag{3}$$

$$\varphi_{ak\sigma} = x_{ak\sigma} a_{k\sigma} + y_{ak\sigma} a_{\bar{k}\sigma}, \tag{4}$$

$$\bar{k} = k + 2k_F, \quad k_F = \pi/2, \quad |x_{ak\sigma}|^2 + |y_{ak\sigma}|^2 = 1,$$

$$a_{k\sigma} = (2M)^{-1/2} \sum_n \exp(-ikn) c_{n\sigma}. \tag{5}$$

The MO is localized on pair m by a unitary transformation [8, 10]:

$$U_{mh} = M^{-1/2} \exp \left[i \left(2m + 1/2 \right) k \right].$$ (6)

The variational parameters $x_{ak\sigma}$, $y_{ak\sigma}$ determine the type of the MO $\varphi_{ak\sigma}$, which corresponds to a one-electron density matrix with perturbed symmetry of period-doubling type. The corresponding variational functions and density matrices relate to states of spin-wave (SW) type, charge-wave (CW) type (deviation from translational symmetry in the diagonal density-matrix elements), or bond-order waves (BOW), spin bond-order waves (SBOW) (symmetry deviation in the nondiagonal density-matrix elements), and also states of mixed type with symmetry deviations in the diagonal and nondiagonal elements (SW-BOW, CW-BOW, etc.). In the nodal representation,

$$f_{ma\sigma} = \sum_n \langle ma\sigma \mid n\sigma \rangle c_{n\sigma},$$ (7)

where the coefficients $\langle ma\sigma \mid n\sigma \rangle$ are defined by (3)-(6).

Formulas (1)-(6) provide the basis for constructing various VLG function types. The VLG functions having w =0 will be denoted by VLG⁰. One can use $\varphi_{ak\sigma}$ corresponding to states of SW, CW, BOW, and SBOW types in (3) to construct VLG functions having the following types: VLG-SW, VLG-CW, VLG-BOW, VLG-SBOW and (for w = 0) VLG⁰-SW, VLG⁰-CW, VLG⁰-BOW, and VLG⁰-SBOW. We put $x_{ak\sigma}=1$, $y_{ak\sigma}=0$, in (4) to get

$$\varphi_{ak\sigma} = \begin{cases} a_{k\sigma}, & a = 1/2, \\ a_{\bar{k}\sigma}, & a = -1/2, \end{cases}$$

which corresponds to the MO in the restricted Hartree-Fock method with completely symmetrical density matrix. For such $\varphi_{ak\sigma}$, which are called plane waves (PW), one can construct two further VLG function types: VLG-PW and VLG⁰-PW. The $x_{ak\sigma}$ and $y_{ak\sigma}$ are expressed in terms of $x_{k\sigma}$ and $y_{k\sigma}$:

$$x_{ak\sigma} = (a + 1/2) x_{k\sigma} + (a - 1/2) y_{k\sigma}^*,$$

$$y_{ak\sigma} = (a + 1/2) y_{k\sigma} - (a - 1/2) x_{k\sigma}, \quad (|k| < k_F)$$ (8)

where the asterisk denotes the complex conjugate.

The type of one-electron function $\varphi_{ak\sigma}$ is determined by the symmetry features of $y_{k\sigma}$ in the substitutions $k \rightarrow -k$, $\sigma \rightarrow -\sigma$ ($x_{k\sigma}$ is unaltered in such substitutions):

SW: $\quad y_{k\sigma} = y_{-k\sigma} = -y_{k,-\sigma}$,

CW: $\quad y_{k\sigma} = y_{-k\sigma} = y_{k,-\sigma}$,

BOW: $\quad y_{k\sigma} = -y_{-k\sigma} = -y_{k\sigma}^* = y_{k,-\sigma}$,

SBOW: $\quad y_{k\sigma} = -y_{-k\sigma} = -y_{k\sigma}^* = -y_{k,-\sigma}$. (9)

For v = 0, we get the GHFM function from the VLG⁰ ones (or simply variational functions with a certain symmetry violation if $\varphi_{ak\sigma}$ is not a GHFM solution):

$$\Psi = \prod_{|k| < k_F} \varphi_{1/2,k\alpha}^- \varphi_{1/2,k\beta}^- \mid 0 \rangle,$$ (10)

whose type is defined by $y_{k\sigma}$ in accordance with (9).

The VLG function used in [8] was of the VLG⁰-BOW type, so the alternat property

$$\langle m, a, \sigma \mid p, \sigma \rangle = (-1)^{p-1} \langle m, -a, \sigma \mid p, \sigma \rangle$$ (11)

for $\langle m, a, \sigma \mid p, \sigma \rangle$ (see (7)) is a consequence of the BOW relations in (9) for $y_{k\sigma}$. The coefficients in (8) and (9) are real for SW and CW but imaginary for BOW and SBOW.

PAIR CORRELATORS FOR VLG FUNCTIONS

The GHFM functions with symmetry deviations (SW, CW, or BOW) lead to nonzero pair correlation functions corresponding to long-range order (SW, CW, or BOW). The long-range order persists after the GHFM functions have been projected on a state with the correct symmetry [3], although such projection leads to zero spin density (for SW), zero charges (for CW), and identical bond orders (for BOW), i.e., the first correlation functions become zero. We have found the following pair correlation functions for functions of VLG^0 type that do not decrease with distance p-q between the atoms p and q:

$$VLG^0 \text{ — SW:} \quad \langle S_z(p) S_z(q) \rangle = 4(-1)^{p-q} \delta^2 (u^2 - v^2)^2, \tag{12}$$

$$VLG^0 \text{ — CW:} \quad \langle Q(p) Q(q) \rangle = 4(-1)^{p-q} \delta^2 (u^2 - v^2)^2, \tag{13}$$

$$VLG^0 \text{ — BOW:} \quad \langle D(p) D(q) \rangle = 4(-1)^{p-q} \Delta^2 (u^2 - v^2)^2, \tag{14}$$

where

$$S_z(p) = (c_{p\alpha}^+ c_{p\alpha} - c_{p\beta}^+ c_{p\beta}), \quad Q(p) = \sum_\sigma c_{p\sigma}^+ c_{p\sigma} - 1, \quad D(p) = \sum_\sigma c_{p\sigma}^+ c_{p+1\sigma} - P; \tag{15}$$

and the parameter δ (spin (charge) wave amplitude) is given by

$$\langle \Psi | c_{q\sigma}^+ c_{q\sigma} | \Psi \rangle = 1/2 + (-1)^q \delta \tag{16}$$

with the GHFM function of (10) having the SW (CW) type, while P and Δ are given by

$$\langle \Psi | c_{q\sigma}^+ c_{q+1\sigma} | \Psi \rangle = P/2 + (-1)^q \Delta \tag{17}$$

with the (10) GHFM function of BOW type. The expressions for the (12)-(14) correlators containing VLG^0 differ from the corresponding ones containing GHFM functions only in the factor $(u^2-v^2)^2 < 1$. The transfer from GHFM to VLG-GHFM reduces the correlators and causes them to become zero in the strong-interaction limit, where the electron Coulomb-repulsion parameters greatly exceed the resonant parameters for interatomic electron jumps, and the contributions to the geminal from the filled and free MO become equal: $u^2 = v^2 = 1/2$. These correlators should become zero for any values of the electron interaction parameters for the exact function.

A spin correlator containing VLG^0-BOW or VLG^0-CW contains only terms that decrease for $p-q \to \infty$ in accordance with $(p-q)^{-2}$; such terms have been deleted on the right in (12)-(14). Other correlators containing VLG^0 of other symmetry types behave similarly: the density-density correlator containing VLG^0-SW and VLG^0-BOW functions and the bond-bond correlator containing VLG^0-SW and VLG^0-CW ones. This reflects the fact that the VLG functions resemble the GHFM ones in establishing their own long-range order, and they constitute an artefact from the viewpoint of the exact solution. For example, it has been found that VLG states [11, 12] show a tendency for a polyene to have alternating bond lengths, which is due to the use in [11, 12] of a VLG^0-BOW function having the correlator of (14) different from zero. On the other hand, GHFM-SW function [12] and a VLG^0-SW one will not lead to bond-length alternation in a polyene, where the latter can be verified.

POLYENE TOTAL ENERGY IN THE VLG-CW

APPROXIMATION

We compare several of the simpler types of VLG function for performance in calculating the ground-state energy for a polyene $(CH)_{2M}$ in an approximation based on an extended Hubbard Hamiltonian:

$$H = -\beta \sum_{n,\sigma} (c_{n\sigma}^+ c_{n+1\sigma} + c_{n+1\sigma}^+ c_{n\sigma}) - \gamma_0 \sum_n c_{n\alpha}^+ c_{n\alpha} c_{n\beta}^+ c_{n\beta} +$$

$$+ \gamma_1 \sum_{n,\sigma,\sigma_1} c_{n\sigma}^+ c_{n\sigma} (c_{n+1\sigma_1}^+ c_{n+1\sigma_1} + c_{n-1\sigma_1}^+ c_{n-1\sigma_1}) - 2\gamma_1 \sum_{n,\sigma} c_{n\sigma}^+ c_{n\sigma} + 2M\gamma_1, \tag{18}$$

where $\beta > 0$ is the electron resonance integral (jump parameter), which is different from zero for adjacent carbon atoms, while γ_0 and γ_1 are the electron Coulomb interaction parameters for electrons correspondingly on the same atom and on adjacent carbon atoms. The penultimate term in (18) describes the electron attraction to the positively charged σ core, while the last term describes the contribution from the repulsion between the positive ionic cores.

The following is the total ground-state energy for a system having a VLG function of (1)-(6) and the Hamiltonian of (18) [13]:

$$E = \sum_m \left[I_m + (1/2) \sum_{n \neq m} (J^{mn} - K^{mn}) \right].$$ (19)

The quantities in (19) here are

$$I_m = \langle 0 | g_m H g_m^+ | 0 \rangle,$$ (20)

$$J^{mn} = \sum_{a,a',b,b'} A_{aa'} A_{bb'} \begin{pmatrix} mm & nn \\ aa' & bb' \end{pmatrix},$$ (21)

$$K^{mn} = \sum_{a,a',b,b'} A_{aa'} A_{bb'} \begin{pmatrix} mn & nm \\ ab & b'a' \end{pmatrix}$$ (22)

(summation is over the two values +1/2 and −1/2 for each subscript a, a', b, b'). The symbols in (20)-(22) are

$$A_{vv} = u^2 + w^2, \quad A_{\mu\mu} = w^2 + v^2, \quad A_{\mu v} = A_{v\mu} = w(u + v)$$
$$(v = 1/2, \ \mu = -1/2)$$ (23)

and

$$\begin{pmatrix} mm' & nn' \\ aa' & bb' \end{pmatrix} = \sum_{pqrs} (pq | rs) \langle ma | p \times q | m'a' \times nb | r \times s | n'b' \rangle,$$ (24)

where

$$(pq | rs) = \delta_{pq} \delta_{rs} [\delta_{pr} \gamma_0 + \gamma_1 (\delta_{p,r-1} + \delta_{r+1})].$$ (25)

We examine the polyene energy for VLG -CW functions of the simplest form with

$$x_{k\sigma} = x, \quad y_{k\sigma} = y \qquad (x^2 + y^2 = 1)$$ (26)

(see (9)) and denote this function type as VLG-CW$_y$. We derive energy expressions for simple VLG function types (VLG-CW, VLG^0-CW, VLG-PW, and so on) and compare the type for performance.

With VLG-CW$_y$, the diagonal contribution is

$$I_m = h + G_m,$$ (27)

where

$$h = 2 \sum_{a,a'} A_{aa'} t_{aa'} - 4\gamma_1, \quad t_{aa'} = 4\beta (x_a x_{a'} - y_a y_{a'})/\pi;$$

$$G_m = u^2 \begin{pmatrix} mm & mm \\ vv & vv \end{pmatrix} + v^2 \begin{pmatrix} mm & mm \\ \mu\mu & \mu\mu \end{pmatrix} + 2w^2 \begin{pmatrix} mm & mm \\ vv & \mu\mu \end{pmatrix} +$$
$$+ 2(w^2 + uv) \begin{pmatrix} mm & mm \\ v\mu & v\mu \end{pmatrix} + 4uw \begin{pmatrix} mm & mm \\ \mu v & vv \end{pmatrix} + 4vw \begin{pmatrix} mm & mm \\ \mu\mu & \mu v \end{pmatrix},$$
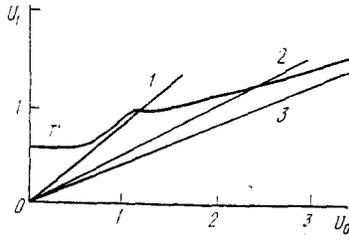$$\mu = -1/2, \quad v = 1/2.$$

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Fig. 1. Phase diagram for an infinity polyene derived in the VLG-CW$_y$ approximation (above the Γ boundary in the plane of U_0 and U_1, the charge-wave state is the ground one, while below Γ, the ground state does not have long-range order): 1) straight line $K = 0$ $(U_0 = 12\,U_1/\pi^2)$; 2) line $U_1 = U_0/2$; 3) line $U_1 = 5\,U_0/12$.

We have from (3)-(6) and (26) for $\langle ma \,|\, n \rangle = \langle n \,|\, ma \rangle$ that

$$\langle 2t \,|\, ma \rangle = (-1)^{m-t}\, P_a/2\pi\,(m - t + 1/4),$$

$$\langle 2t + 1 \,|\, ma \rangle = (-1)^{m-t}\, Q_a/2\pi\,(m - t - 1/4), \tag{28}$$

$$P_a = x_a + y_a, \quad Q_a = y_a - x_a.$$

The following sums over (m, n) must be calculated to derive the total energy of (19) via (24)-(28):

$$\left(\begin{matrix} mm \\ aa' \end{matrix} \,\middle|\, \begin{matrix} mm \\ bb' \end{matrix} \right) = \frac{\gamma_0}{6}\, S_1 + \frac{2\gamma_1}{\pi^2}\, S_2,$$

$$\sum_{n \neq m} \left(\begin{matrix} mn \\ aa' \end{matrix} \,\middle|\, \begin{matrix} nm \\ bb' \end{matrix} \right) = \frac{\gamma_0}{12}\, S_1, \quad \sum_{n \neq m} \left(\begin{matrix} mm \\ aa' \end{matrix} \,\middle|\, \begin{matrix} nn \\ aa' \end{matrix} \right) = \frac{\gamma_0}{12}\, S_1 + \frac{\gamma_1}{\pi^2}\, (\pi^2 - 4)\, S_2, \tag{29}$$

$$S_1 = P_a P_{a'} P_b P_{b'} + Q_a Q_{a'} Q_b Q_{b'}, \quad S_2 = P_a P_{a'} Q_b Q_{b'} + Q_a Q_{a'} P_b P_{b'}.$$

We put

$$u = \cos\varphi \cos\chi, \quad v = \sin\varphi \cos\chi, \quad w = (1/\sqrt{2})\sin\chi, \quad x = \cos\theta, \quad y = \sin\theta \tag{30}$$

and use (19)-(23) with (29) to get an expression for the total energy $E = E(\varphi, \chi, \theta)$ per electron:

$$\varepsilon(\varphi, \chi, \theta) = (1/2M)\, E(\varphi, \chi, \theta).$$

The energy is defined by this expression for $\theta = 0$ for VLG-PW functions, or with $\chi = \theta = 0$ for VLG^0-PV.

Analytic and numerical studies on $\varepsilon(\varphi, \chi, \theta)$ have been made with various values of $U_0 = \gamma_0/\beta$ and $U_1 = \gamma_1/\beta$, which have shown that in the (U_0, U_1) plane there is a boundary Γ (Fig. 1) below which $(U_1 < U_1(\Gamma))$ the VLG^0-PW states are favored by energy (the minimum in $\varepsilon(\varphi, \chi, \theta)$ occurs for $\chi = \theta = 0$). Above Γ $(U_1 > U_1(\Gamma))$, the VLG-CW$_y$ state having $\chi \neq 0$, $\theta \neq 0$ is favored by energy. In the VLG^0-PW state, $\varepsilon(\varphi, 0, 0)$ has a minimum at $\varphi = \varphi_0$, where φ_0 is defined by

$$\operatorname{tg} 2\varphi_0 = -\pi K/24, \qquad K = U_0 - 12U_1/\pi^2. \tag{31}$$

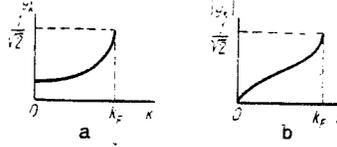For small U_0 and U_1 $(U_0, U_1 \ll 1)$, we have

Fig. 2. Dependence of y_k on the quasi-momentum k for: a) GHFM-SW (CW); b) GHFM-BOW.

$$\varepsilon(\varphi_0, 0, 0)/\beta = -4/\pi + U_0/4 - 2U_1/\pi^2 - \pi K^2/288 + O(K^4). \tag{32}$$

The same expansions for ε have been derived in [8] (for $U_1 = 0$) and in [14] (for $U_1 \neq 0$).

The VLG^0-PW solution of (31) has been examined in the region U_0, $U_1 \leqslant 1$ for $U_1 > U_1(\Gamma)$ by means of a second-derivative matrix calculated for the point $(\varphi, \chi, \theta) = (\varphi_0, 0, 0)$:

$$\begin{pmatrix} B & 0 & 0 \\ 0 & C & D \\ 0 & D & F \end{pmatrix}, \quad B = \frac{\partial^2 \varepsilon}{\partial \varphi^2}, \quad C = \frac{\partial^2 \varepsilon}{\partial \chi^2}, \quad D = \frac{\partial^2 \varepsilon}{\partial \chi \partial \theta}, \quad F = \frac{\partial^2 \varepsilon}{\partial \theta^2}. \tag{33}$$

The simple expression for B is

$$B = (1/3\pi) \cos 2\varphi_0 (48 + \pi^2 K^2/12) > 0.$$

The analytic-calculation system REDUCE-2 [15] has been used to derive expressions for C, D, and F. In the region U_0, $U_1 \leqslant 1$, there are critical values U_1^{cr} for which VLG^0-PW becomes unstable:

$$U_1^{cr} = 6\pi/(4\pi^2 - 11) \qquad (U_0 = 0)$$
$$U_1^{cr} = 3\pi/2(\pi^2 - 5) \qquad (U_0 = 12U_1/\pi^2). \tag{34}$$

The U_1^{cr} at which the VLG^0-PW state vanishes is close to the $U_1(\Gamma)$, for which the VLG^0-PW state ceases to be the ground one.

In the region U_0, $U_1 \gg 1$, one can determine the relative magnitudes of the energy minima for the VLG states only by direct energy calculation. The solution containing $(\varphi_0, 0, 0)$ remains stable, although it may be higher in energy than the (φ, χ, θ) solution. We have found for U_0, $U_1 \gg 1$ that the Γ line approaches the following straight line asymptotically:

$$U_1 \simeq 0.41 U_0. \tag{35}$$

This numerical result is readily explained by comparing the energies for the VLG^0-PW and VLG-CW$_y$ states in the limit U_0, $U_1 \gg 1$; for VLG^0-PW we have [8]

$$\varepsilon(\text{VLG}^0 - \text{PW}) \simeq U_0/12. \tag{36}$$

For VLG-CW$_y$, we get numerically, as in GHFM for the SW state for U_0, $U_1 \gg 1$) that

$$\varepsilon(\text{VLG} - \text{CW}_y) \simeq U_0/2 - U_1. \tag{37}$$

We equate (36) and (37) to get

$$U_1(\Gamma) = (5/12)U_0 \simeq 0.416 U_0. \tag{38}$$

DISCUSSION

It has been shown in [8, 9] and here that all the VLG functions (including the simple VLG^0-PW ones) give a description of correlation effects in polyene chains better than do the GHFM ones. We have examined the relative energies for various VLG-type states on the simple

VLG-CW$_y$ example. For $U_1 < U_1(\Gamma)$, the VLG^0-BOW state energy is less than the VLG-CW$_y$ value, which coincides in this parameter region with the VLG^0-PW state. For U_0, $U_1 \ll 1$, the energy difference between these states is small:

$$\varepsilon \,(\text{VLG} - \text{CW}_y) - \varepsilon \,(\text{VLG}^0 - \text{BOW}) = \varepsilon \,(\text{VLG}^0 - \text{PW}) - \varepsilon \,(\text{VLG}^2 - \text{BOW}) = O\,(K^4)$$

In the range $U_1 > U_1(\Gamma)$, the VLGF-CW$_y$ state has energy lower than VLG^0-BOW described in [8]. The forms of the Γ boundary separating the state having nonzero CW amplitude differ considerably from the phase diagram derived in the GHFM method [2], and also from numerical calculations by Monte Carlo methods [16] and from the renorm-group method [17, 18] on account of our approximation for x_k and y_k in (26), which describes the behavior of these quantities incorrectly for $k = k_F$. The k dependence of y_k in the self-consistent GHFM for SW states is [2]

$$y_k = \sin\left(\frac{1}{2}\arcsin\left(\gamma_0\delta/\sqrt{\gamma_0^2\delta^2 + 4\beta^2\cos^2 k}\right)\right);\qquad(39)$$

while for CW states, γ_0 must be replaced by $4\gamma_1 - \gamma_0$, while δ is a variational-function parameter. Figure 2a shows y_k for the GHFM-CW and SW functions; Fig. 2b gives $|y_k|$ for the BOW function obtained in the self-consistent GHFM.

Figure 2a shows that $y_k = $ const represents y_k closely for large U_0 and U_1, where $y_k \simeq 1/\sqrt{2}$, but describes it incorrectly for small and medium U_0 and U_1. That situation has been found previously [11, 19] for VLG^0-BOW functions. With $|y_k| = \sin\theta_k$, $\theta_k = \lambda k$, where λ is a variational parameter, it has proved impossible to describe the system energy correctly for $U_0 \to 0$, whereas $\theta_k = (1/2)\arctan(\lambda \, tg\, k)$ with any λ gives $\theta_{k_F} = \pi/4$, which enables one to describe the energy correclty for $U_0 \to 0$.

Then the choice of one-electron basis can have a marked effect on the VLG behavior, as is evident also in the asynmptotic $U_1(\Gamma)$ for large U_0 and U_1. For U_0, $U_1 \gg 1$, the position of Γ is defined from comparing the energies of VLG-CW$_y$ in (37) and VLG^0- PW in (36). When one compares the VLG-CW$_y$ energy with the energy of the VLG^0-BOW state [8]

$$\varepsilon \,(\text{VLG}^0 - \text{BOW}) \sim 1/U_0 \simeq 0, \qquad U_0 \gg 1$$

we get an equation for the Γ boundary:

$$U_1(\Gamma) = U_0/2.$$

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